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Extended Equation-of-State for Dichlorodifluoromethane (CCl_2F_2)

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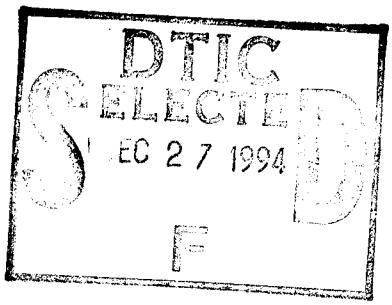

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A new equation-of-state for decomposed CCl_2F_2 (dichlorodifluoromethane) has been developed. This new equation-of-state is based upon equilibrium composition calculations of the components and possible products of CCl_2F_2 and utilizes tables of thermochemical properties for each of the gas species. Since the thermochemical property tables had an upper temperature limit of 6,000 °K, these tables first had to be extended to cover the temperature range of interest. The new equation-of-state covers the pressure range of 0.1 to 100,000 bar and the temperature range from 200 to 30,000 °K, and with certain limitations, up to 500,000 °K. The methods used to extend the thermochemical tables and to determine the equilibrium gas composition are described.

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Dichlorodifluoromethane	High Temperature	Decursor

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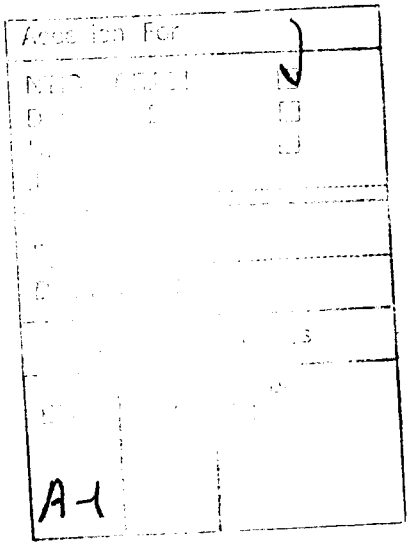

SUMMARY

The JANAF Thermochemical Tables contained the 41 species possible as the result of the decomposition of dichlorodifluoro-methane (CCl_2F_2). The thermochemical properties needed to determine the equilibrium properties of the gas mixture were given up to a temperature of 6,000 K. To allow determination of the gas mixture properties at temperatures higher than 6,000 K, the JANAF tables were duplicated and then extended to 30,000 K. There were six species that were not calculated with standard methods and required special handling. These species therefore are not as accurate in the thermodynamic properties as the rest of the species. But as there should only be a small fraction of those six species present, the effect on the mixture properties should be minimal.

The JANAF tables only carried the first positive ionization specie for each of the elements present (F, Cl, and C). At the higher temperatures and lower pressures of the equilibrium analysis, large quantities of these ions were found to be present. This indicated that additional ionization levels of each specie were required, until there was not a significant amount of the highest ionization level present. Using the same method as that used for calculating the singly ionized elements, tables for the second, third, and fourth ionization levels of the three elements present were created. These additional nine species (F^{++}, F^{+++}, F^{++++}, Cl^{++}, Cl^{+++}, Cl^{++++}, C^{++}, C^{+++}, and C^{++++}) then were included in the equilibrium analysis, bringing the total number of species under consideration to 50 and allowing the equilibrium properties of the decomposed CCl_2F_2 gas mixture to be evaluated at temperatures as high as 30,000 K. For monatomic species, the data was calculated through 500,000 K while considering 31 species.

The equation-of-state for the gas mixture consisting of decomposed CCl_2F_2 has been examined. Only an equilibrium calculation is feasible with the information currently available. As many as 50 species must be considered with temperatures as high as 30,000 K and pressures as low as 0.1 bar. The solution method for determining the equilibrium mixture was to use the thermochemical data to calculate an equilibrium constant for a series of reactions. Each reaction then generated a nonlinear equation involving the equilibrium

constant and the species partial pressures. The resulting 50 equations were solved simultaneously to determine the amount of each specie present. With the amount of each specie known, the mixture properties at those conditions were readily calculated.

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SECTION 1
INTRODUCTION

In recent years, the Defense Nuclear Agency (DNA) has placed the emphasis of its airblast research program on high overpressure effects over real, rather than ideal, surfaces. Real surface effects include thermal and mechanical modifications of the blast wave. Thermal modification of the blast wave creates the nuclear blast precursor. Mechanical modifications can be caused by surface roughness, irregular terrain, entrained dust, and by the pressure of high-density layers above the ground surface. Such high-density layers can occur naturally from snowfall or wind deposition of vegetation debris. High-density layers also may be produced by the blow-off of the soil surface by high-energy X-rays from a nuclear explosion.

To simulate the blast modification effects of high-density layers, DNA attempted to use various porous solid materials. However, there were significant difficulties encountered in calculating the behavior of these solid materials in high-pressure blast environments. For this reason, DNA chose to perform a number of blast experiments using layers of heavy gases rather than porous solids.

For practical reasons, dichlorodifluoromethane (CCl_2F_2) was selected for use in several of these heavy gas-layer experiments. To perform calculations of such experiments, it is necessary to have an equation of state for CCl_2F_2. There was a limited amount of equation-of-state data, but there were significant voids in this data base. Logicon R&D Associates (RDA) identified deficiencies in the data base and the preliminary equation-of-state and then embarked upon a project to extend the available data base and create an equation-of-state suitable for use in the temperature and pressure regimes of these experiments. This report describes this project.

SECTION 2
PROBLEM DESCRIPTION AND APPROACH

To properly model the blast experiments, it is necessary to determine the properties of the gas used. CCl_2F_2 was placed in the experiment and was the initial gas present. However, while CCl_2F_2 is a relatively stable compound under normal conditions, it will decompose rapidly at temperatures above 2,000 K. Such temperatures are reached quickly during the experiment. Thus, the properties normally associated with CCl_2F_2 are valid during the initial portion of the experiment, but thereafter should be the properties of the gas mixture consisting of decomposed CCl_2F_2. In order to evaluate these properties, the composition of the gas mixture must be known. If the mixture is not in equilibrium, then the rates of all the reactions needed to produce the various gas species present must be known and the properties will be a function of time as well as pressure and temperature. As there are dozens of gas species involved, and very few of the reaction rates are known, the only practical recourse is to assume that the gas mixture is in equilibrium. The properties then will no longer be a function of time. The validity of the equilibrium assumption must be evaluated separately.

The preliminary CCl_2F_2 equilibrium calculations were performed by Science Applications International Corporation (SAIC). These had two difficulties. The first was that an insufficient number of species was carried in the analysis. While some of the heavier molecules that were missing had a noticeable effect on the mixture composition, the results were not wildly wrong. However, at the higher temperature end, not enough ionized species were allowed, resulting in a significantly different result. Whether these differences in composition caused significant variations in mixture properties was not examined in great detail. However, a quick look did indicate noticeable differences in the properties at high temperatures. The other problem was that the calculations were done with two different codes (CET89 and EIONY) for different temperature regimes (Ref.1). The valid temperature regions did not overlap, and actually had a significant gap between them. The results were blended together, but the blended region has an anomaly that does not correspond to a real molecule or mixture, indicating a problem with the assumptions or method used to combine the results.

After evaluating the preliminary equation-of-state, Logicon RDA determined that an improved one would be necessary to properly analyze the blast experiments. To determine the equilibrium properties of the gas mixture consisting of decomposed CCl_2F_2, certain thermochemical properties must be known. These include the enthalpy, Gibbs free energy, and heat capacity of each individual gas specie. The equilibrium composition of a gas mixture can be calculated by different techniques, though each will require essentially the same properties of the individual component species. The common source for obtaining these properties is the JANAF Thermochemical Tables (Refs. 2 and 3). These tables provide several thermochemical properties of many gas species. The difficulty is that these tables have a maximum temperature of 6,000 K. In general, it is possible to use the same calculational procedures and input as those used to generate the JANAF tables and thus duplicate those tables. The calculations need not stop at the arbitrary limit of 6,000 K, but can be extended to higher temperatures (Ref. 4). Care must be used not to ignore some input terms that may have been discarded due to the limited temperatures of the JANAF tables.

Using extended tables, the equilibrium constants have been calculated for all the reactions needed to determine the composition of the decomposed CCl_2F_2 gas mixture. By evaluating the many simultaneous equations that relate the equilibrium constants with a reaction, the gas composition can be calculated and then the properties determined (Ref. 5). This has been done for a wide range of temperatures and pressures using the EQUIL code, a new code developed by Logicon RDA specifically for this analysis.

CCl_2F_2 also is known by the generic names refrigerant-12 and chlorofluorocarbon-12 and by several trade names including Freon-12, Fluorocarbon-12, Genetron-12, Isotron-12, and Ucon-12.

SECTION 3
EXTENDING JANAF TABLES

In order to solve the equilibrium composition for CCl_2F_2, knowledge of certain thermochemical properties of each constituent specie must be available. Species that are possible to be present, and therefore must have properties available, are listed below.

CCl_2F_2	C(s)	C_2	e^-	F^-
CF_4	CCl	C_3	C_2^-	F^+
CCl_4	CCl_2	C_4	CF^+	F^{++}
$CClF_3$	CCl_3	C_5	CF_2^+	F^{+++}
CCl_3F	CF	C_2Cl_2	CF_3^+	F^{++++}
Cl_2	CF_2	C_2Cl_4	Cl^-	C^-
Cl	CF_3	C_2Cl_6	Cl^+	C^+
F_2	ClF	C_2F_2	Cl^{++}	C^{++}
F	ClF_3	C_2F_4	Cl^{+++}	C^{+++}
C	ClF_5	C_2F_6	Cl^{++++}	C^{++++}

The JANAF Thermochemical Tables provide values of various thermodynamic functions for ideal gases. These values are a function of temperature (T) only and therefore are independent of pressure. All values are normalized by the universal gas constant (R_u).

There are four general classes of gaseous molecules in the JANAF tables: monatomic, diatomic, linear polyatomic, and nonlinear polyatomic. Among the gases required for the CCl_2F_2 analysis, there also are six special cases that use variations of the standard evaluation methods. These special cases will be discussed individually. There are a few errors in the input data as listed in the 1985 JANAF tables. These will be covered in the next section. The last section discusses monatomic gases at extremely high temperatures.

The thermodynamic functions of interest are the normalized molar heat capacity at constant pressure ($C_p^\circ(T)/R_u$), normalized enthalpy ($[H^\circ(T)-H^\circ(298.15\ K)]/R_uT$), normalized Gibbs free

energy (-[$G^\circ(T)$-$H^\circ(298.15\ K)$]/R_uT), and normalized entropy ($S^\circ(T)/R_u$). Throughout this document, these normalized functions will be referred to as heat capacity, enthalpy, Gibbs energy, and entropy.

The relationships between the thermodynamic functions and the partition function are:

$$Q(T) = \text{Partition Function}$$

$$\frac{-[G^\circ(T) - H^\circ(0K)]}{R_uT} = \ln Q(T) \qquad \textit{(Gibbs energy)}$$

$$\frac{[H^\circ(T) - H^\circ(0K)]}{R_uT} = T\frac{d\ln Q(T)}{dT} \qquad \textit{(Enthalpy)}$$

$$\frac{S^\circ(T)}{R_u} = T\frac{d\ln Q(T)}{dT} + \ln Q(T) \qquad \textit{(Entropy)}$$

$$\frac{C_p^\circ(T)}{R_u} = T^2\frac{d^2\ln Q(T)}{dT^2} + 2T\frac{d\ln Q(T)}{dT} \qquad \textit{(Heat capacity)}$$

The partition function usually is broken down into components associated with each energy: translation (Q_t), electronic (Q_e), rotation (Q_r), and vibration (Q_v). In addition, there may be an additional term associated with corrections for anharmonic vibrations (Q_a). Translation is not coupled to any of the other terms and so may be freely separated from the rest. The other terms are classified as the internal partition function (Q_i).

$$Q(T) = Q_t(T)\ Q_i(T)$$

where

$$Q_i(T) = \sum_j \left(Q_e(T)\right)_j \left(Q_r(T)\right)_j \left(Q_v(T)\right)_j \left(Q_a(T)\right)_j$$

The individual thermodynamic properties then can also be separated. For example, the heat capacity at constant pressure (C_p)

$$\frac{C_p^\circ(T)}{R_u} = \left(\frac{C_p^\circ(T)}{R_u}\right)_t + \left(\frac{C_p^\circ(T)}{R_u}\right)_i$$

The internal partition function also is frequently separated into individual terms, although cross-coupling terms do not always make it proper to do so. It is valid, however, when only one of the partition functions has more than one term, such as when there are three electronic states, but only the ground rotation and vibration states. Thus, the above equations become

$$Q(T) = Q_t(T)\ Q_e(T)\ Q_r(T)\ Q_v(T)\ Q_a(T)$$

and

$$\frac{C_p^\circ(T)}{R_u} = \left(\frac{C_p^\circ(T)}{R_u}\right)_t + \left(\frac{C_p^\circ(T)}{R_u}\right)_e + \left(\frac{C_p^\circ(T)}{R_u}\right)_r + \left(\frac{C_p^\circ(T)}{R_u}\right)_v + \left(\frac{C_p^\circ(T)}{R_u}\right)_a$$

3.1 MONATOMIC GASES.

This is the easiest class to evaluate. Additionally, this class contains the largest body of experimental data needed to support the calculations. The abundance of the necessary input data and the simplicity of the molecules and thus the calculations, make the results for the monatomic gases the most accurate beyond 6,000 K, especially for the extremely high temperatures.

For the monatomic gases, there are only two contributors to the thermodynamic functions: translation and electronic. The normalized contributions from translation for the monatomic gases (and all the gases, for that matter) are:

$$\frac{-[G^\circ(T) - H^\circ(0K)]}{R_u T} = \frac{3}{2}\ln M_r + \frac{5}{2}\ln T + \ln\frac{k}{p^\circ}\left(\frac{2\pi k}{Nh^2}\right)^{\frac{3}{2}}$$

$$\frac{[H^\circ(T) - H^\circ(0K)]}{R_u T} = \frac{5}{2}$$

$$\frac{S^\circ(T)}{R_u} = \frac{3}{2}\ln M_r + \frac{5}{2}\ln T + \frac{5}{2} + \ln\frac{k}{p^\circ}\left(\frac{2\pi k}{N_A h^2}\right)^{\frac{3}{2}}$$

$$\frac{C_p(T)}{R_u} = \frac{5}{2}$$

In the above Gibbs energy and entropy equations, M_r is the molecular weight (grams/mole) of the specie. The last term is a function only of the pressure (p°) and constants (k is the Boltzmann constant, N_A is Avogadro's number, and h is the Planck constant). At one bar, it evaluates to -3.6517. (Note that this term must be evaluated using cgs units.)

The contributions for the electronic states are:

$$Q(T) = \sum_i g_i e^{\frac{-c_2\epsilon_i}{kT}}$$

$$\frac{-[G^\circ(T) - H^\circ(0K)]}{R_u T} = \ln\sum_i g_i e^{\frac{-c_2\epsilon_i}{kT}}$$

$$\frac{[H^\circ(T) - H^\circ(0K)]}{R_u T} = \frac{c_2}{T}\frac{\sum_i \epsilon_i g_i e^{\frac{-c_2\epsilon_i}{kT}}}{\sum_i g_i e^{\frac{-c_2\epsilon_i}{kT}}}$$

$$\frac{S^{\circ}(T)}{R_u} = \frac{c_2}{T}\frac{\sum_i \epsilon_i g_i e^{\frac{-c_2\epsilon_i}{kT}}}{\sum_i g_i e^{\frac{-c_2\epsilon_i}{kT}}} - \ln \sum_i g_i e^{\frac{-c_2\epsilon_i}{kT}}$$

$$\frac{C_p(T)}{R_u} = \frac{c_2^2}{T^2}\left[\frac{\sum_i \epsilon_i^2 g_i e^{\frac{-c_2\epsilon_i}{kT}}}{\sum_i g_i e^{\frac{-c_2\epsilon_i}{kT}}} - \left(\frac{\sum_i \epsilon_i g_i e^{\frac{-c_2\epsilon_i}{kT}}}{\sum_i g_i e^{\frac{-c_2\epsilon_i}{kT}}}\right)^2\right]$$

For the above equations, ϵ_i is in units of cm^{-1}. The value of the second radiation constant [$c_2 = k/(hc)$, where c is the speed of light in a vacuum] is 1.438786 cm-K. The input for a specie includes molecular weight, number of energy levels, and for each energy level, the energy of the level (ϵ_i) and the degeneracy of the level (g_i). In the 1985 edition of the JANAF tables (Ref. 2), the number of levels given has been reduced to only those that affect the results at or below 6,000 K. The previous edition (Ref. 3) carried many more energy levels.

An alternate set of thermochemical tables has been published (Ref. 6). In this set of tables, most of the monatomic species have been carried to 10,000 K and some to 20,000 K. However, detailed examination of the tables and comparing them with the results of this analysis indicate that this source only carried the same number of energy levels as the 1985 JANAF tables, but carried the calculations to higher temperatures. This results in a significant error above 6,000 K compared to using the terms in the 1971 JANAF edition. (The 1971 edition did combine many of the higher energy levels into much fewer terms, but this provides an adequate approximation for temperatures up to 30,000 K.) Since this

alternate source was shown to provide incorrect answers for part of its temperature range, it was rejected as a source of comparison for temperatures above those in the JANAF tables.

Since the 1985 JANAF tables did not contain nearly enough energy levels for accuracy above 6,000 K, another source was needed. The 1971 JANAF tables contain a much more complete input, but since some of the higher levels were combined, it was unclear what effect this might have on very high temperatures. Therefore, the energy levels and degeneracies were obtained from published atomic energy level data (Ref. 7). All energy levels were carried up to the ionization limit for each monatomic specie.

All the monatomic species used for the CCl_2F_2 analysis were compared with the JANAF tables for the temperatures up to 6,000 K, and checked to within three on the last published digit, which is an error less than 0.01 percent. The calculations were then carried out to 30,000 K. Subsequently, a request was made to have results at even higher temperatures, so the calculations were run again, going up to a temperature of 500,000 K, but at much larger temperature steps than the 100 K increments used up to 30,000 K (refer to Section 3.7).

During the course of the equilibrium calculations which use the extended JANAF tables, it was observed that at low pressures (0.1 bar) and high temperatures (30,000 K) there were significant amounts of the singly ionized atoms present (F^+, Cl^+, C^+), which were the highest ionization levels considered at that time. Additional ionization levels were added until the species did not contribute anything to the mixture properties. This eventually resulted in including up to the fourth ionization species (F^{++++}, Cl^{++++}, C^{++++}). Even more ionization species were added to give proper mixtures at the extremely high temperature requested (500,000 K). Though these multiply ionized species were not present in the JANAF tables, all the necessary energy levels and degeneracies were available (Ref. 7) to create the tables using the same method as was used for the singly ionized atoms. Also present was the ionization level of the species, used to calculate the heat of formation, which is needed for the equilibrium calculation.

3.2 DIATOMIC GASES.

The calculations for a diatomic gas are, in general, the most complex since there are frequently multiple vibrational states in addition to multiple electronic states. For this analysis, the translational partition function was separated, but the internal partition function remained combined. Thus, all the cross-component terms were properly carried throughout the computations.

The translational partition function is the same as it is for the monatomic gases. Each individual state of the electronic partition function is also the same for monatomic gases, but must be combined with the other internal partition function values at that state before the summation over all states can be performed. The electronic, rotational, vibrational, and anharmonic partition functions for diatomic molecules are given below.

$$Q_e(T) = g e^{-\frac{c_2 \epsilon}{T}}$$

$$Q_r(T) = \frac{T}{\sigma c_2 (B_e - \frac{1}{2}\alpha_e)}$$

$$u \equiv \frac{c_2}{T}(\omega_e - 2\omega_e x_e)$$

$$Q_v(T) = \frac{1}{1 - e^{-u}}$$

$$Q_a(T) = \frac{1}{u}\left(\frac{8B_e}{\omega_e}\right) + \frac{1}{e^{u}-1}\left(\frac{\alpha_e}{B_e}\right) + \frac{2 x_e u}{(e_u-1)^2}$$

In these equations, the values for σ (symmetry number), B_e (the rotational constant), α_e (first-order rotation vibration interaction constant), ω_e (vibrational fundamental for infinitesimal amplitude), and x_e (anharmonicity correction) are spectroscopic data that are part of the

known input for each gas specie and given in the JANAF tables. With the values for each Q known, the terms required for the Gibbs free energy, enthalpy, entropy, and heat capacity can be evaluated using the basic relationship between the thermodynamic functions and the partition function. These are combined for the four different partition functions into the values for the internal partition function for each state, and then the values for all the states are combined into the total contribution from the internal partition function.

All the diatomic species used for the CCl_2F_2 analysis were compared with the JANAF tables for temperatures up to 6,000 K, and, except for two species that will be discussed under the special cases section, all checked to within 0.1 percent. This included species that had multiple electronic states, multiple vibrational states, and one specie with multiple electronic and vibrational states. The calculations then were carried out to 30,000 K. The higher temperature results for the diatomic species are not as reliable as for the monatomic gases as there were generally no higher electronic states provided for input. This is somewhat offset by the expectation that, at the higher temperatures where these electronic states might become important, there will not be enough of the diatomic species present to make a significant contribution to the global gas thermochemical properties.

3.3 LINEAR POLYATOMIC GASES.

The linear polyatomic gases are treated essentially the same as diatomic gases; however, with some adjustments. The corrections for anharmonic vibrations were ignored. The number of vibrational degrees of freedom (N_v) was adjusted for the number of atoms (N) in the molecule and the linear nature of the molecule ($N_v = 3N-5$). The third change was made because the spectroscopic input data combined terms. Also, of the species under consideration, none had multiple states associated with any individual partition function. Therefore, the contributions for each partition function were split and calculated independently of the other partition functions, without having an effect upon the final thermochemical property values. Since multiple terms were not present, the contributions by the rotational partition function were calculated using the approximation given in the 1985 edition of the JANAF tables.

$$B \equiv \frac{B_e - \alpha_e}{2}$$

$$\left(\frac{C_p^{\circ}(T)}{R_u}\right)_r = 1 + \frac{1}{45}\left(\frac{c_2 B}{T}\right)^2$$

$$\left(\frac{[H^{\circ}(T) - H^{\circ}(0K)]}{R_u T}\right)_r = 1 - \frac{1}{3}\left(\frac{c_2 B}{T}\right) - \frac{1}{45}\left(\frac{c_2 B}{T}\right)^2$$

$$\left(\frac{S^{\circ}(T)}{R_u}\right)_r = 1 - \ln\left(\frac{c_2 B \sigma}{T}\right) - \frac{1}{90}\left(\frac{c_2 B}{T}\right)$$

$$\left(\frac{-[G^{\circ}(T) - H^{\circ}(0K)]}{R_u T}\right)_r = -\ln\left(\frac{c_2 B \sigma}{T}\right) + \frac{\frac{c_2 B}{T}}{3} + \frac{\left(\frac{c_2 B}{T}\right)^2}{90}$$

There were only six species that fell into this category. One of them, C_3, was calculated as a special case. The other five species all checked to within 0.1-percent accuracy when compared with the JANAF tables for 0 K through 6,000 K. As with the diatomic species, the farther beyond 6,000 K the calculations are carried, the less confidence in the thermodynamic properties. However, even to a greater extent than for the diatomics, at temperatures where properties are less certain, it is expected that there will not be enough of the polyatomics around to affect the global thermodynamic properties of the mixture, even if the values for the polyatomics are wildly off.

3.4 NONLINEAR POLYATOMIC GASES.

The nonlinear polyatomic gases are treated the same as the linear polyatomic gases with two adjustments. The number of vibrational degrees of freedom (N_v) was adjusted in a slightly different manner for the number of atoms in the molecule (N) to reflect the nonlinear nature of the molecule (N_v = 3N-6). The other change was made because the molecule now has a significant moment of inertia along all three axes. Again, of the species under consideration, none had multiple states associated with any individual partition function, so each partition function was split from and calculated independently of the other partition functions. With the nonlinear molecule, the contributions by the rotational partition function were calculated using the equations given in the 1985 edition of the JANAF tables.

$$\left(\frac{C_p^{\circ}(T)}{R_u}\right)_r = \frac{3}{2}$$

$$\left(\frac{[H^{\circ}(T) - H^{\circ}(0K)]}{R_u T}\right)_r = \frac{3}{2}$$

$$\left(\frac{S^{\circ}(T)}{R_u}\right)_r = \frac{3}{2} + \frac{1}{2}\ln\left(\frac{\pi\sigma}{I_A I_B I_C}\right)$$

$$\left(\frac{-[G^{\circ}(T) - H^{\circ}(0K)]}{R_u T}\right)_r = \frac{1}{2}\ln\left(\frac{\pi\sigma}{I_A I_B I_C}\right)$$

$I_A\ I_B\ I_C$ is the product of the principal moments of inertia of the molecule. Of the species that fell into this category, two were special cases. The other species all checked to within 0.1-percent accuracy when compared with the JANAF tables for 0 K through 6,000 K. As

with the linear polyatomic species, the further beyond 6,000 K the calculations are carried, the less confidence in the thermodynamic properties. However, as stated for the linear polyatomics, at temperatures where properties are less certain, it is expected there will not be enough of the polyatomics around to affect the global thermodynamic properties of the mixture, even if the values for the polyatomics are wildly off.

3.5 SPECIAL CASES.

There were six special cases among the species considered for the CCl_2F_2 mixture analysis. Five were alluded to in the above descriptions while the sixth is a condensed specie and cannot be evaluated using ideal gas methods. The six species are C(s), Cl_2, F_2, C_3, C_2Cl_6, and C_2F_6. The Cl_2 and F_2 caused the most concern of all the species that required special treatment, since there was the greatest likelihood for significant amounts of these species to be present under high-temperature and high-pressure conditions. Large errors in the properties of these two species would have the greatest chance of causing noticeable errors in the calculated properties of the CCl_2F_2 mixtures. These six exceptions to the standard calculational methods employed will be discussed individually, with a description of exactly what was done to arrive at an adequate evaluation of the thermochemical properties.

C(s): This is condensed carbon, otherwise known as graphite. It is a solid specie and cannot be evaluated using methods discussed for the various varieties of ideal gases. Values for the heat capacity beyond 6,000 K were not readily available. This most likely has to do with the C(s) melting point being somewhere around 4,300 K. Therefore, the heat capacity for temperatures above 6,000 K was assumed to be constant at the JANAF table value at 6,000 K. The other thermochemical properties then can be evaluated from the heat capacity and the other known values at 6,000 K. All the properties for C(s) at 6,000 K and below were set to be the same as in the 1985 JANAF tables. Above 6,000 K, the following equations were used.

$$C_p^{\circ}(T) = C_p^{\circ}(6{,}000\,K) = 29.946$$

$$[H°(T) - H°(298.15K)] = [H°(6{,}000K) - H°(298.15K)] + C_p°(T)\,(T - 6{,}000)$$

$$\frac{-[G°(T) - H°(298.15K)]}{T} = \frac{-[G°(6{,}000K) - H°(298.15K)]}{T} +$$

$$C_p(T)\left[\left(\frac{298.15}{T} - \frac{298.15}{6{,}000}\right) + (\ln T - \ln 6{,}000)\right]$$

$$S°(T) = \frac{[H°(T) - H°(298.15K)]}{T} + \frac{-[G°(T) - H°(298.15K)]}{T}$$

These equations match the JANAF table values at 6,000 K and provide a smooth transition to the extended values.

Related to the properties of C(s), but associated with gaseous carbon in the JANAF tables, is the column for log $K_p(T)$, which, for C, is the same as the vapor pressure ($P_c(T)$) of C(s). The vapor pressure can be determined by the following equation (Ref. 8).

$$\ln P_c(T) = \frac{-E_0(C)}{R_u T} - \left(\frac{G°(T) - H°(0K)}{R_u T}\right)_C + \left(\frac{G°(T) - H°(0K)}{R_u T}\right)_{C(s)}$$

(Note that "log" is logarithm base 10 and "ln" is logarithm base e.) Using this equation in conjunction with the extended tables for C(s) and C, the vapor pressure for solid carbon can be determined. This is needed in the CCl_2F_2 analysis to determine the upper bound on the amount of carbon gas allowed in the system.

Cl_2: The thermochemical property values derived for Cl_2 by the analysis did not match the JANAF tables. But it was different from the rest of the special cases in that a cause for the

discrepancy was not determined. Also, the error was somewhat odd. While none of the properties match the JANAF values, extracting the value of the partition function, Q, from the tables produced the same value as the analysis was calculating. Somehow, the terms related to Q had a discrepancy which, while not off wildly, was noticeable. And yet another specie with similar levels of vibrational and electronic states matched the tables perfectly, indicating that the analysis code was functioning properly. It is possible that there is an error in the input data as published in the JANAF tables, but, if so, it has not yet been found.

Therefore, the JANAF table results at 6,000 K and below were declared correct and used. For temperatures above the JANAF tables, the results of the analytical calculation were used, but the values were adjusted with an offset so they matched the values in the JANAF tables at 6,000 K.

F_2: The F_2 calculation for the 1985 JANAF tables was done in a very different manner than for the 1971 JANAF tables. Instead of using a single vibrational manifold and calculating the summation, each vibrational state was enumerated and spectroscopic constants provided. The details of this special evaluation were not obtained and the table could not be duplicated. It should be noted that the new table contained very different results from the previous table.

Since the 1985 JANAF table was deemed correct, it was used for the values at and below 6,000 K. Above that temperature, the old values of input (from the 1971 JANAF tables) were used for the calculation, but were adjusted with an offset so that the values matched the 1985 tables at 6,000 K.

C_3: The discrepancy in the values for C_3 caused the least amount of concern, as this molecule is truly a special case. In an attempt to get the results to better match certain experiments, the evaluation of the vibrational states of C_3 was arbitrarily limited in the JANAF results. Historically, there has been much discussion of the correct properties for C_3, mainly concerned with calculations in a pure carbon environment. Other equation values have been proposed that more accurately reflect experimental results in such environments (Refs. 9, 10).

Of the various proposed solutions, the one by Strauss and Thiele (Ref. 9) has produced generally favorable comparisons with experiment. Other proposed solutions also closely approximate this solution. Therefore, their proposed thermochemical properties, instead of the JANAF properties, have been selected for use in this analysis. The equations were set up and the results agree with those published by Strauss and Thiele to within 0.01 percent for the temperature ranges in the reference. The equations used contributions from translational, bending-rotational, and vibrational sources. The translational terms are the same as for the monatomic species and the vibrational terms are the same for the diatomic species. The bending-rotational partition function is given by the following equations.

$$U(\theta) = \frac{hc}{48B_e}\left(\frac{\nu_0}{c}\right)^2 \theta^2 + \frac{h^2c^2\sigma}{576B_e^2}\left(\frac{\nu_0}{c}\right)^4 \theta^4$$

$$Q_{br} = \frac{1}{48}\left(\frac{kT}{hcB_e}\right)^2 \int_0^{\pi} e^{\frac{U(\theta)}{kT}} \sin\theta \, d\theta$$

Experimental measurements provide $\nu_0/c = 55.5511$ cm^{-1} and $hc\sigma = 0.001062$ cm. θ is the variable of integration. The property terms for the bending-rotational terms are given by the equations for the relationships between the thermodynamic functions and the partition function.

C_2Cl_6: The input data for C_2Cl_6 indicate that the calculation includes additional terms for internal rotation. This is a special case that did not appear to warrant an attempt to evaluate it, since it is expected that very little of this large molecule will be present at temperatures of 6,000 K and above.

The solution for this molecule was to use the JANAF tables for temperatures of 6,000 K and below. For temperatures above this, the calculation ignored the internal rotation, while adjusting the value of $I_AI_BI_C$ to provide the correct value at 298 K. The adjusted value was 1.125×10^{-108}, changed from the published value of 9.145×10^{-112}. The results were adjusted by an offset to match the JANAF values at 6,000 K.

C_2F_6: The input data for C_2F_6 indicate that the calculation includes additional terms for torsion. Like C_2Cl_6, this is a special case that did not appear to warrant an attempt to evaluate it, since it is expected that very little of this large molecule will be present at temperatures of 6,000 K and above.

The solution for this molecule was to use the JANAF tables for temperatures of 6,000 K and below. For temperatures above this, the calculation ignored the internal rotation, while adjusting the value of $I_A I_B I_C$ to provide the correct value of Q_p at 298 K. The adjusted value was 8.275×10^{-112}, changed from the published value of 6.005×10^{-113}. The results were adjusted by an offset to match the JANAF values at 6,000 K.

3.6 JANAF TABLE INPUT DATA ERRORS.

During the course of calculating the results for the many species considered for analyzing the CCl_2F_2 mixtures, there were several species that did not match the results in the 1985 JANAF tables. Five of those species required the special treatment listed above. The rest of the discrepancies were resolved by making adjustments to the input data (there appeared to be definite difficulty with the correct value of σ, the symmetry number). As the results using the corrected input agree with the JANAF tables, those corrections have been declared correct. The corrections are listed below.

- F_2 - under vibration level 7 (v=7), the value of B_v is listed as 0.7484, but is really 0.7844. (Note that this correction was not actually used, as the calculation was done as a special case instead.)
- CF_2^+ - σ is not listed. The correct value is 2.
- CF_3^+ - σ is listed as 1, but the correct value is 6.
- CCl_4 - σ is listed as 2, but the correct value is 12.

3.7 EXTREMELY HIGH TEMPERATURES.

While the original intent was to extend the JANAF tables to around 12,000 K, they were eventually extended to 30,000 K so that mixture properties could be obtained at these high temperatures. It then was found that it would be useful to have the mixture properties for temperatures beyond 30,000 K, all the way to tens of electron volts (eV). As 20 eV corresponds to about 230,000 K, this was very much beyond the current temperature level of the JANAF tables. It was decided to attempt calculation of the equation-of-state at the higher temperatures by running the JANAF tables to these extremely high temperatures. As the multiatomic molecules would be well beyond a reasonable temperature, only monatomics were used for this very much elevated temperature region.

Some interaction between the equation-of-state calculations and the JANAF table calculations did occur. The pressures in the equation-of-state calculations ranged from 0.1 bar through 100,000 bar. The highest temperature to be used in the mixture calculation was 500,000 K, corresponding to 43.1 eV. The first results showed that the mixture consisted of electrons and the fourth ionization levels of all three atoms (Cl^{++++}, F^{++++}, and C^{++++}). This indicated that not enough ionization levels were being considered. Therefore, tables were created for the following additional species:

Cl^{+5}	Cl^{+8}	Cl^{+10}	F^{+6}	C^{+5}
Cl^{+6}	Cl^{+9}	F^{+5}	F^{+7}	C^{+6}
Cl^{+7}				

Carbon only went through six ionization levels as there are only six electrons on the carbon atom. While fluorine has nine electrons, the atomic energy levels available (without doing additional research) only were through the seventh ionization level. Data available for chlorine was through the tenth ionization level.

Using the energy level data for the additional 11 species and the same method used for the second through fourth ionization levels, the equivalent JANAF tables were created for the

additional ionization levels. The tables are, of course, at best only as accurate as the energy level data. While these data are, in general, experimentally determined, some values are estimated. While such estimates do not have much influence at lower temperatures, for these extremely high temperatures it is possible that there is some significant error introduced.

SECTION 4
EQUATION-OF-STATE CALCULATIONS

The calculations performed to determine the properties of the gas mixture (Ref. 11) of decomposed CCl_2F_2 have two major assumptions. First, as previously stated, this is an equilibrium calculation. The assumption is that it took an infinite amount of time to reach this state. The reality is that it most likely took significantly less time to reach a condition that is very close to this equilibrium state. In fact, to be applied to the hydrodynamic calculation as anticipated, that near equilibrium condition may have to be reached within microseconds.

The other assumption is that this is an ideal gas. That is, there are no real gas effects present. The enthalpy, entropy, and free energy are a function of temperature only and *not* a function of pressure. This assumption most certainly is false over some range of the temperatures and pressures being calculated, specifically at low temperature and high pressure. At 400 K and 100,000 bar, pressure has a significant effect on the gas mixture and properties. An estimate at the point at which real gas effects become significant will be made. If a noticeable portion of the hydrodynamic code calculations use results within the area of real gas effects, the analysis should be reevaluated. Along with the real gas effects, condensed species, with the exception of solid carbon, have been ignored. Thus, at 400 K and 100,000 bar, most likely there would be a pool of liquid. That possibility is not recognized in these calculations.

It also should be noted that this effort was started as an independent check on the equilibrium results that already had been calculated. As such, it was decided to perform the calculations using a different code and a different method from those used in the previous calculations. This code (EQUIL) was written specifically for this analysis.

4.1 MIXTURE SPECIES.

For the equilibrium mixture calculation, all the species that are to be part of the composition must be determined prior to the calculation since the component species properties are required to calculate the composition. If a specie is not really present, then it will be calculated as being a very small part of the mixture. The preliminary calculations of the mixture composition performed by SAIC using the CET89 code considered 35 possible species, of which 10 were ions. There were 41 possible species with properties in the JANAF tables. All 41 species were considered in the EQUIL calculations and are listed below.

CCl_2F_2	C	ClF	C_2Cl_4†	CF_2^+
CF_4	C(s)	ClF_3	C_2Cl_6†	CF_3^+
CCl_4	CCl	ClF_5†	C_2F_2	Cl^-
$CClF_3$†	CCl_2	C_2	C_2F_4	Cl^+
CCl_3F	CCl_3	C_3	C_2F_6†	F^-
Cl_2	CF	C_4	e^-	F^{+}†
Cl	CF_2	C_5	C_2^-	C^-
F_2	CF_3	C_2Cl_2	CF^+	C^+
F				

† = not considered in CET89 calculations

In addition, after several calculations were done at higher temperatures and lower pressures, there was a significant amount of singly ionized atoms present. This implied that additional ionization levels should be considered. Consequently, the following nine species were added to the list of mixture species considered, after first creating equivalent JANAF tables for them.

Cl^{++}	Cl^{++++}	F^{+++}	C^{++}	C^{++++}
Cl^{+++}	F^{++}	F^{++++}	C^{+++}	

4.2 JANAF TABLES ABOVE 6,000°K.

The JANAF Thermochemical Tables contain the species property data for the range from 0 K through 6,000 K. The mixture properties are required at higher temperatures. Though the originally estimated limit was 10,000 K to 12,000 K, it eventually was decided that temperatures as high as 30,000 K might be needed. Therefore, an effort was made to extend the JANAF tables to the higher temperature limit.

The tables were duplicated and then extended to 30,000 K (Section 3). There were a few species that required special handling, but overall the process was straightforward, if a bit time consuming. While this extension is somewhat uncertain for the polyatomic species with no information about electronic levels, it was anticipated that there would not be very many of the polyatomic molecules present. The most prevalent specie class, the monatomics, can be calculated to a relatively high accuracy as long as the atomic energy levels for the specie are known, as they are for the atoms involved in the CCl_2F_2 mixture. All 50 species being considered in the CCl_2F_2 mixture now have properties data from 0 K through 30,000 K in 100 K increments.

4.3 REACTIONS AND EQUILIBRIUM CONSTANTS.

The reactions considered in this analysis are of the form

$$a_1 A_1 + a_2 A_2 + a_3 A_3 \rightleftarrows b_1 B_1 + b_2 B_2 + b_3 B_3$$

where

A_i = the reactant molecule

B_i = the product molecule

a_i = number of reactant molecules

b_i = number of product molecules

There can be, at most, three different reactant species and three different product species. The equilibrium constant for a given reaction can be calculated from knowing the Gibbs free

energy and the heat of formation of the species involved in the reaction (Ref. 8). The equilibrium constant for this reaction is defined in terms of the partial pressures where P_i denotes the partial pressure of specie i.

$$K_p = \frac{P_{B_1}^{b_1} P_{B_2}^{b_2} P_{B_3}^{b_3}}{P_{A_1}^{a_1} P_{A_2}^{a_2} P_{A_3}^{a_3}}$$

The equilibrium constant, K_p, may be computed from the partition function of each specie participating in the reaction, Q, and the heat of formation at 0 K (E_0).

$$\Delta E_0 = b_1 E_0(B_1) + b_2 E_0(B_2) + b_3 E_0(B_3) - a_1 E_0(A_1) - a_2 E_0(A_2) - a_3 E_0(A_3)$$

$$\ln K_p = \frac{-\Delta E_0}{R_u T} + b_1 \ln Q(B_1) + b_2 \ln Q(B_2) + b_3 \ln Q(B_3) - a_1 \ln Q(A_1) - a_2 \ln Q(A_2) - a_3 \ln Q(A_3)$$

The heat of formation is given in the JANAF tables and the free-energy function may be calculated from the Gibbs free energy in the same tables.

$$Q = e^{\ln Q} = e^{\frac{-[G°(T) - H°(0K)]}{R_u T}}$$

In this equation-of-state analysis, the species' partial pressures were not the natural variable to use in solving for the species. A more appropriate variable is the specie mole fraction. The partial pressure, P_i, is related to the mole fraction, x_i, and the total system pressure, P, by

$$P_i = P \times x_i$$

The equilibrium constant can then written as

$$K_p = \frac{x_{B_1}^{b_1} x_{B_2}^{b_2} x_{B_3}^{b_3}}{x_{A_1}^{a_1} x_{A_2}^{a_2} x_{A_3}^{a_3}} P^{b_1+b_2+b_3-a_1-a_2-a_3}$$

As an example, consider the following reaction.

$$2\,CCl_2F_2 \rightleftarrows CCl_4 + CF_4$$

The equilibrium constant then provides the relationship between the species' partial pressures.

$$K_p = \frac{P_{CCl_4} P_{CF_4}}{P^2_{CCl_2F_2}}$$

Writing this in terms of the mole fractions gives

$$K_p = \frac{x_{CCl_4} x_{CF_4}}{x^2_{CCl_2F_2}}$$

For the example equilibrium condition, K_p is only a function of the species involved and the temperature. The system pressure has cancelled out of this particular reaction and is not a factor. If these three species are the only species present in the system, the mole fractions are readily determined. Some sample results are shown below.

K_p	CCl_2F_2	CCl_4	CF_4
0.10	0.612	0.194	0.194
0.25	0.500	0.250	0.250
1.0	0.333	0.333	0.333
4.0	0.200	0.400	0.400
10.	0.136	0.432	0.432

4.4 CONDENSED SPECIES.

There is only one condensed specie allowed in this analysis, solid carbon, denoted by C(s). Actually, if any other condensed specie were present under the analysis conditions, the analysis would be in error. This most certainly will occur at the very low temperature and very high pressure conditions.

When solid carbon is present, the amount of gaseous carbon present is set by the vapor pressure of the solid carbon. The vapor pressure of C above C(s) as determined by the third law of thermodynamics is

$$\ln (P_v)_C = \frac{-E_0(C)}{R_u T} - \left(\frac{G^\circ - H_0^\circ}{R_u T}\right)_C + \left(\frac{G^\circ - H_0^\circ}{R_u T}\right)_{C(s)}$$

where the heat of formation of C(s) has been defined as 0.0 (Ref. 11). This relationship between C and C(s) is available directly from the JANAF tables. The last column under C is labeled "Log K_f" and is the logarithm base 10 of the vapor pressure of C. Note that this simple relationship does *not* hold between this column and the larger carbon molecules such as C_2 and C_3. However, because this is an equilibrium analysis, the values calculated for C_2 and C_3 *will* be the vapor pressure of those molecules. Condensed species have no gas pressure and so must not be counted when calculating mole fractions in the reaction pressure equations.

4.5 MIXTURE COMPOSITION.

To determine the composition of the mixture, a series of equations must be written, one for each specie that is being considered. Most of these equations will be reaction equations, which eventually will relate equilibrium constants to species mole fractions. Another advantage of performing an equilibrium analysis is that it does not matter if the reaction equations are the ones that actually occur. The equilibrium assumption means that however roundabout an equation is written, the solution will be the same. All that is necessary is to

make sure there are no redundant equations present; there must not be more than one way to get to a product. For example, a CF_2 equation can be written as

$$CF_2 \rightleftarrows C + F_2$$

or it can be written as

$$CF_2 \rightleftarrows C + 2F$$

But *both* forms cannot be present. (The above reactions assume that both F and F_2 are present in the system.) Refer to Appendix B for the nominal set of reaction equations used to solve for the Freon mixture.

In addition to the reaction equations, the other equations needed are the summation of the atoms Cl, F, and C. When ions are present, there also is the summation of electric charge. Using the previous example with CCl_2F_2, CCl_4, and CF_4 as the only three species present, when the mole fractions were determined for various values of K_p, the following two equations were implied;

$$2 = 2\,x_{CCl_2F_2} + 4\,x_{CCl_4}$$

$$2 = 2\,x_{CCl_2F_2} + 4\,x_{CF_4}$$

However, the carbon summation equation,

$$1 = x_{CCl_2F_2} + x_{CCl_4} + x_{CF_4}$$

does not provide any new information as long as all the possible species each contain exactly one carbon atom. It also should be noted that since the number of moles present is not constant, the number on the left side of the summation equations needs to be multiplied by the ratio of the original number of moles over the current number of moles. Since mass is conserved, this also is the ratio of the mixture molecular weight and the CCl_2F_2 molecular weight. For the simple case above, this ratio was 1.

When the reaction set is complete, there will be one equation for each specie. For the species under analysis, that means that there are 50 simultaneous equations to be solved. But 46 of those equations are nonlinear, making finding a solution a nontrivial effort. Three main methods have been used in this analysis. All involve iteration to a solution and require a "reasonable" guess as to the correct solution before the iterations will converge.

The first technique is to linearize the reaction rate equations. A standard solver then can be used to solve the 50 linear equations. The linear solution is fed back into the nonlinear equations and the next guess at the solution is made. If the original guess was close enough, the iteration will converge to the answer. If not, the process will fail. An additional difficulty with the linearized method is that as some species are present only in very small mole fractions, the linear matrix can readily become singular, or nearly so. To remove the singularity, the reaction and the specie must be removed and all species strictly dependent upon the removed specie also must be removed. But if the reaction set was written such that a specie with a very small presence connects a specie with a large presence into the system, the reaction set must be rewritten instead. With so many species present and the mole fractions of the species varying significantly over the solution range, this was a daunting task. This solution technique is no longer being used.

The second method is to solve the nonlinear equation set. This appears to work better, even if sometimes only minimally. Once the reaction equations have been written, the next step is to assign each reaction to a specie for solution. Of course, the specie must be involved in the reaction assigned to it for solution. It should be noted that the summation equations should be used to solve for a specie with a large mole fraction or numerical difficulties can arise. Starting from the initial solution guess, each equation is solved by iteration. If the initial guess was close enough, the solution will generally converge. The solution at the previous condition is used as the guess for the solution at a nearby pressure and temperature. However, as the relative amount of the various species changes, the equations that should be assigned to each specie change. Sometimes determining the correct assignment is straightforward, but other times it requires some trial and error to determine the proper

reaction assignments. In spite of the difficulties, this technique appears faster than using the linearized method.

But there still were computational regions where both methods became excruciatingly slow to converge. Finally, a third solution method was formulated. This technique separates the linear from the nonlinear equations. The nonlinear equations then are reformulated with a change of variable to produce another set of linear equations. These two sets of linear equations have a nonlinear relationship between them. First one set of equations is solved. The results are fed into the second set and then those equations are solved. Since the assignment of the species to one set or another essentially is arbitrary, the linear independence of the equations in each set is no longer automatic. Several checks must be made during the assignment to ensure that both sets of equations will have a solution. Also, reactions 1 through 26 in Appendix B were changed so that all species were in equilibrium with their constituent atoms. This method solves at about the same speed as the other methods when their convergence is fast. However, when convergence slows down, this method only takes two to five times longer instead of orders of magnitude longer for the other two techniques. In fact, this method was so fast that all cases were rerun according to it and the answers agreed with previously obtained answers.

Under some conditions, the number of species has been reduced from the 50 listed above. Below 6,000 K, the nine multiply ionized species are not present in significant quantities and are removed from the reaction set, allowing for a faster iteration to solution. And below 3,200 K, there are no ionized species present in perceptible amounts, so the 20 ionized species are not used. For uniformity of printout, any specie not present is assigned a mole fraction of 1.0×10^{-150}.

4.6 MIXTURE PROPERTIES.

Once the mole fractions of the species have been determined, it is easy to calculate the mixture properties needed. The molecular weight is simply the summation of the species molecular weights multiplied by their mole fraction:

$$\overline{M} = \sum_{i=1}^{n} f_i \overline{M}_i$$

And knowing the molecular weight, pressure, and temperature, the density of an ideal gas is easily found from the perfect gas law:

$$P = \rho R T$$

The internal energy of a mixture is determined by summing over the mole fraction energies of the individual species:

$$E = \sum_{i=1}^{n} x_i E_i$$

The heat capacity at constant pressure and the heat capacity at constant volume also can be calculated in a similar manner. The ratio of these specific heats, γ, then can be obtained. The enthalpy, if needed, is also calculated this way.

4.7 ELEVATED TEMPERATURES.

It was suggested subsequently that it would be useful to have the mixture properties for temperatures beyond 30,000 K, all the way to tens of electron volts (eV). As 20 eV corresponds to about 230,000 K, this was very much beyond the current temperature level of the equation-of-state analysis. As the multiatomic molecules would be well beyond a reasonable temperature limit for their existence, only the monatomics were used for this very much elevated temperature region.

For this elevated temperature regime, the highest temperature to be used in the mixture calculation was 500,000 K, corresponding to 43.1 eV. The first results showed that the mixture consisted of electrons and the fourth ionization levels of all three atoms (Cl^{++++}, F^{++++}, and C^{++++}). This indicated that not enough ionization levels were being considered. Therefore, tables were created for the following additional species:

Cl^{+5}	Cl^{+8}	Cl^{+10}	F^{+6}	C^{+5}
Cl^{+6}	Cl^{+9}	F^{+5}	F^{+7}	C^{+6}
Cl^{+7}				

Carbon only went through six ionization levels as there are only six electrons on the carbon atom. While fluorine has nine electrons, the atomic energy levels available (without doing additional research) were only through the seventh ionization level. Data was available for chlorine through the tenth ionization level.

The results of the equation-of-state calculations for temperatures higher than 30,000°K should be used with caution. In examining the mole fractions, two things became apparent. At 500,000 K and low pressures, most of the chlorine was Cl^{+10}, most of the fluorine was F^{+7}, and most of the carbon was C^{+6}, all of which are the highest ionization levels considered. The carbon is no problem as there are no additional ionization levels for it. However, this indicates that for a proper answer under these conditions, even higher ionization levels of chlorine and fluorine must be used. At the high-pressure conditions at 500,000 K, the most prominent species were Cl^{+8}, F^{+7}, and C^{++++}. Here, while the chlorine and carbon are acceptable, it still appears that additional ionization levels of fluorine are required. As these extreme temperatures were not vital, the effort was not expended to obtain the energy level data required for additional ionization levels of fluoride.

At the low temperature end of the elevated temperatures, 30,000 K, the results were compared with those obtained using the 50 species given earlier. At 0.1 bar, even though the elevated temperature calculation used only monatomic species, the error in density was 0.025 percent and the error in internal energy was 0.061 percent, both quite satisfactory. However, at 100,000 bar, the solutions diverged quite significantly. The error in density was 38.1 percent and for the internal energy, it was 5.93 percent. So at pressures above about 1,000 bar at 30,000 K with the elevated temperature species, the error in the mixture properties begins to become significant. It is unclear just where the curve of significant error should be drawn, but it would appear that at 50,000 K and 100,000 bar there would, in the real world, probably

be a noticeable amount of diatomic molecules present, which were not allowed in the evaluation.

4.8 REAL GAS EFFECTS.

The ideal gas approximation has been used in Section 4.6 to calculate the thermodynamic mixture properties of Freon over a wide range of temperature and pressure. At sufficiently high pressure, real gas effects become important and will influence both the mixture composition and the mixture thermodynamic properties. The corresponding states method (see, for example, Chapter 4 of Ref. 13) is easily applied to a mixture of given composition to determine the influence of pressure upon the mixture properties. However, calculating the mixture composition when the Gibbs free energy of each component is pressure-dependent is a tedious procedure and is beyond the scope of this effort. Instead, we shall provide an estimate of the pressure and temperature regime in which the ideal gas assumption is accurate and define a pressure boundary above which the ideal gas assumption becomes questionable.

The most convenient indicator of real gas behavior is the deviation of the compressibility factor Z [$Z = P/(\rho RT)$] from a value of unity. We shall arbitrarily set the boundary between ideal gas and real gas behavior at $Z = 1.10$. That is, we set the boundary where the compressibility factor has increased by 10 percent from the perfect gas value of unity. This boundary between the real and ideal gas regime is shown in terms of the reduced pressure and temperature in Figure 4-1. The corresponding states table of compressibility from Breedveld (Table 1A-3 of Ref. 11) was used with a constant value of $Z = 1.10$ to generate Figure 4-1.

To determine the boundary between real and ideal gas behavior in terms of the physical coordinates (i.e., P and T), we use the pseudocritical method (Chapter 4 of Ref. 14) to define the critical point properties for the mixture. These values are given by:

$$T_{cm} = \frac{\sum_i x_i T_{c_i}}{1 - x_c^*}$$

$$P_{cm} = \frac{(1 - x_c^* T_{cm}}{\sum_i x_i T_{c_i} / P_{c_i}}$$

where T_{cm} and P_{cm} are the pseudocritical mixture values for temperature and pressure. The mole fraction for each i component of the mixture is x_i and x_c^* is the mole fraction of the condensed carbon. T_{ci} and P_{ci} are the critical point temperature and pressure of each component. The reduced temperature and pressure are defined by:

$$T_R \equiv \frac{T}{T_{cm}} \quad \text{and} \quad P_R \equiv \frac{P}{P_{cm}}$$

Using the ideal gas calculation to define the mixture composition and the above equations for the pseudocritical values, T_{cm} and P_{cm}, and for the reduced coordinates, T_R and P_R, Figure 4-1 may be replotted in terms of the physical coordinates in Figure 4-2. The tables of Reference 12 only extend out to a reduced temperature of fifty. Extrapolating the curve of Figure 4-1 to larger values of T_R gives the dashed line of Figure 4-2.

Therefore, in the pressure and temperature regime that lies below the curve of Figure 4-2, the ideal gas assumption should be valid and the present results may be used with confidence. However, at pressures that lie above the curve, real gas effects will limit the accuracy and caution is advised.

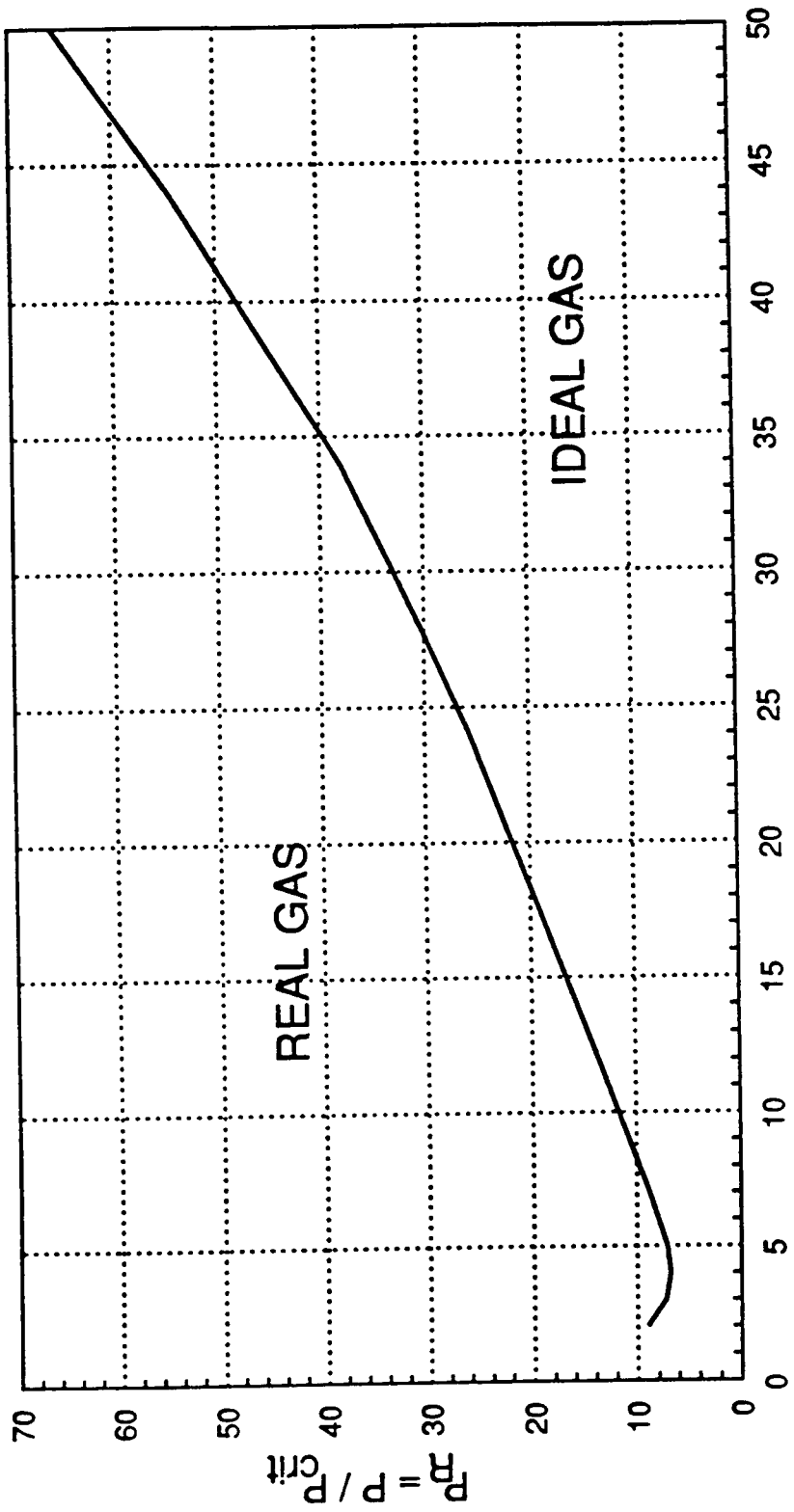

Figure 4-1. Boundary between real gas and perfect gas regimes in terms of reduced coordinates for Z = 1.10.

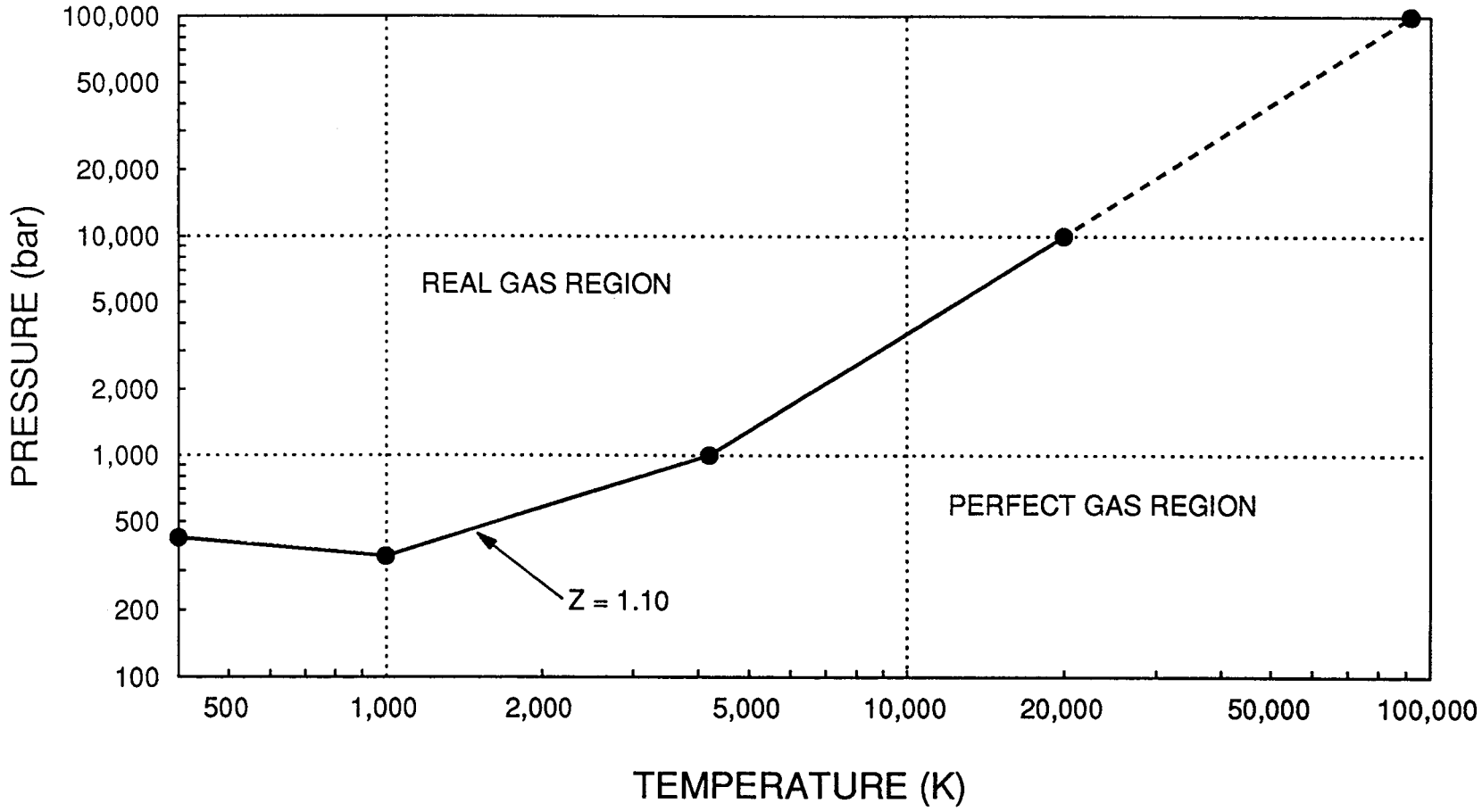

Figure 4-2. Equillibrium CCl_2F_2 real gas regions.

4.9 SOLUTION SPACE.

When it was determined that a grid of mixture properties as a function of pressure and temperature would be needed, a set of points was chosen. The pressure would range from 0.1 bar through 100,000 bar with 6 approximately equally-ratioed values within each decade (1.0000, 1.5157, 2.2894, 3.4641, 5.0000, 7.0000) for a total of 37 pressures. The following temperatures selected:

Every 400 K between 400 and 10,000 K
Every 1,000 K between 11,000 and 20,000 K
25,000 K
30,000 K
50,000 K
100,000 K
200,000 K
500,000 K

This made for a total of 1,517 data points.

During the evaluation of some of the shock tube experiment results, the data in the above grid were included in the analysis. When a simple bilinear interpolation was used on that data, the results showed significant distortion of certain values, most notably density, in the spaces between the grid points. (See Figure 4-3.) This was additional impetus to complete a table with finer grid points than those above. While resolving certain numerical difficulties with the computer code, the finer grid table was completed. It covers the same pressure range, but has 18 values per decade (1.0000, 1.1487, 1.3195, 1.5157, 1.7411, 2.0000, 2.2894, 2.6207, 3.0000, 3.4641, 4.0000, 4.4721, 5.0000, 5.4772, 6.0000, 7.0000, 8.0000, 9.0000) for a total of 109 pressures. The following temperatures were used:

Every 100 K between 200 and 10,000 K
Every 200 K between 10,200 and 15,000 K
Every 500 K between 15,500 and 20,000 K
Every 1,000 K between 21,000 and 30,000 K

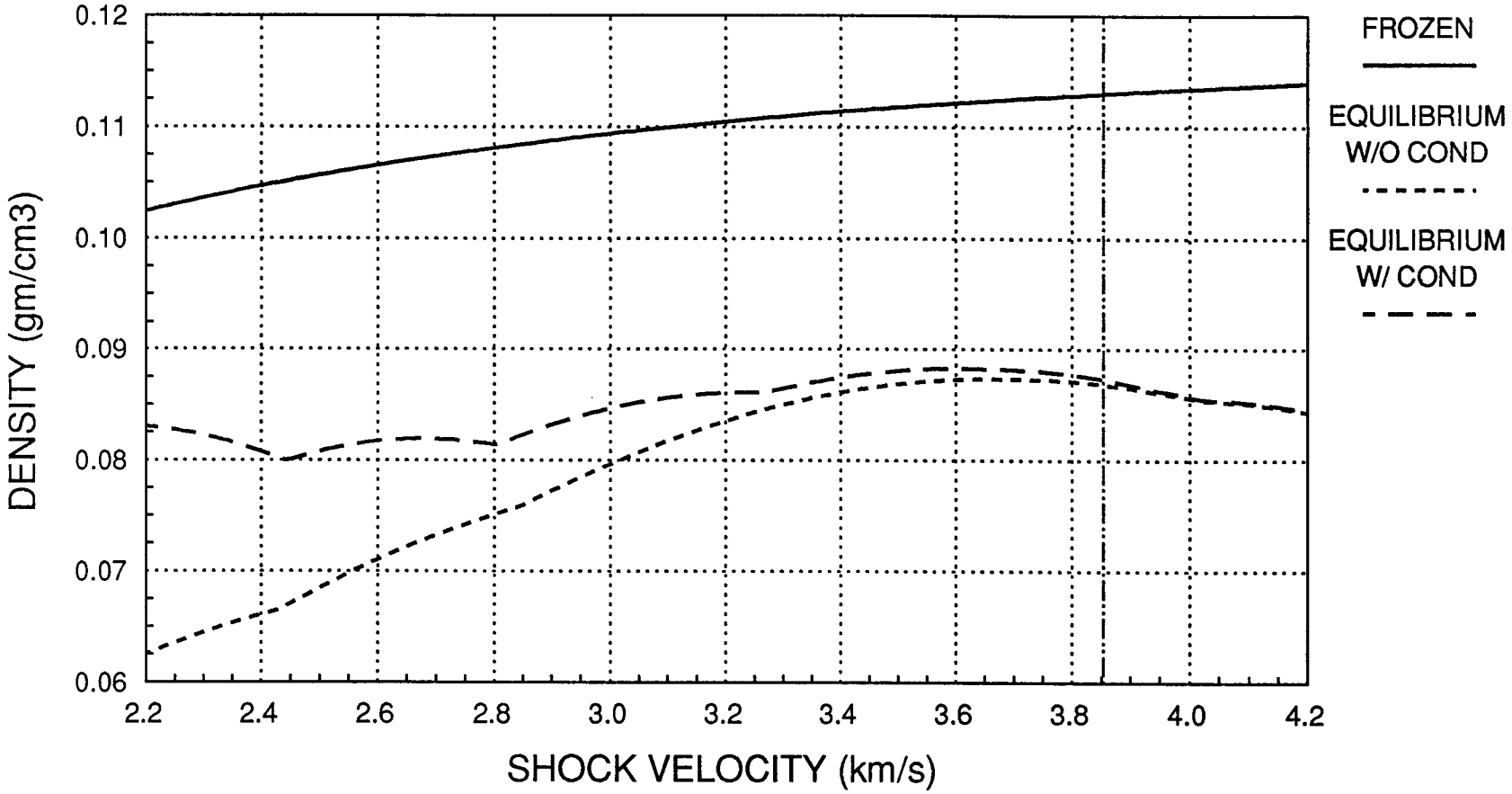

Figure 4-3. Shock tube calculations.

Every 2,000 K between 32,000 and 50,000 K

Every 5,000 K between 55,000 and 100,000 K

Every 10,000 K between 110,000 and 200,000 K

Every 20,000 K between 220,000 and 500,000 K

Thus, there were 20,601 data points in this finer grid.

Both tables were sent to Dr. James R. Barthel at the S-Cubed Division of Maxwell Laboratories, Inc. on PC-formatted floppy disks.

SECTION 5

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APPENDIX A

TABLES FOR MONATOMIC, DIATOMIC, LINEAR POLYATOMIC, AND NONLINEAR POLYATOMIC SPECIES

The following four tables (Tables A-1 to A-4) show sample comparisons between the JANAF tables and the calculated values. There is one representative molecule from each of the four categories of molecules. While the range from 0 K through 6,000 K is complete, only the major temperature increments from 6,000 K through 30,000 K are shown. The JANAF tables are from Reference 1.

Table A-1. JANAF Table for Monatomic Specie: Cl.

a. Chlorine (Cl) $cl_1(g)$

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = p° = 0.1 MPa

	J K^{-1}mol^{-1}			kJ mol^{-1}			
T/K	C_p°	S°	$-[G^\circ-H^\circ(T_r)]/T$	$H^\circ-H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	Log K_f
0	0.	0.	INFINITE	-6.272	119.621	119.621	INFINITE
100	20.788	142.175	184.104	-4.183	120.244	115.476	-60.319
200	21.079	156.636	167.161	-2.105	120.813	110.482	-28.855
250	21.450	161.378	165.547	-1.042	121.066	107.869	-22.538
298.15	21.838	165.189	165.189	0.	121.302	105.306	-18.449
300	21.852	165.325	165.190	0.040	121.311	105.207	-18.318
350	22.202	168.720	165.457	1.142	121.553	102.504	-15.298
400	22.467	171.703	166.055	2.259	121.795	99.766	-13.028
450	22.644	174.361	166.833	3.387	122.035	96.998	-11.259
500	22.744	176.752	167.708	4.522	122.272	94.203	-9.841
600	22.781	180.905	169.571	6.800	122.734	88.546	-7.709
700	22.692	184.411	171.448	9.074	123.172	82.813	-6.180
800	22.549	187.432	173.261	11.337	123.585	77.019	-5.029
900	22.389	190.079	174.986	13.584	123.972	71.174	-4.131
1000	22.233	192.430	176.615	15.815	124.334	65.288	-3.410
1100	22.089	194.542	178.150	18.031	124.675	59.367	-2.819
1200	21.959	196.458	179.597	20.233	124.997	53.416	-2.325
1300	21.843	198.211	180.963	22.423	125.300	47.438	-1.906
1400	21.742	199.826	182.253	24.602	125.589	41.438	-1.546
1500	21.652	201.323	183.475	26.772	125.863	35.417	-1.233
1600	21.573	202.718	184.635	28.933	126.124	29.379	-0.959
1700	21.504	204.024	185.737	31.087	126.374	23.325	-0.717
1800	21.443	205.251	186.788	33.234	126.612	17.256	-0.501
1900	21.389	206.409	187.790	35.375	126.840	11.175	-0.307
2000	21.341	207.505	188.749	37.512	127.058	5.081	-0.133
2100	21.298	208.545	189.667	39.644	127.265	-1.023	0.025
2200	21.260	209.535	190.548	41.772	127.463	-7.136	0.169
2300	21.226	210.479	191.394	43.896	127.650	-13.259	0.301
2400	21.195	211.382	192.208	46.017	127.827	-19.389	0.422
2500	21.167	212.246	192.992	48.135	127.992	-25.526	0.533
2600	21.142	213.076	193.749	50.250	128.147	-31.670	0.636
2700	21.119	213.874	194.480	52.364	128.290	-37.820	0.732
2800	21.099	214.641	195.186	54.474	128.421	-43.974	0.820
2900	21.080	215.381	195.870	56.583	128.541	-50.133	0.903
3000	21.063	216.096	196.532	58.690	128.649	-56.297	0.980
3100	21.047	216.786	197.174	60.796	128.746	-62.463	1.052
3200	21.032	217.454	197.798	62.900	128.832	-68.633	1.120
3300	21.019	218.101	198.403	65.002	128.908	-74.804	1.184
3400	21.007	218.728	198.992	67.104	128.974	-80.979	1.244
3500	20.995	219.337	199.564	69.204	129.031	-87.155	1.301
3600	20.985	219.928	200.122	71.303	129.081	-93.332	1.354
3700	20.975	220.503	200.665	73.401	129.124	-99.511	1.405
3800	20.966	221.062	201.195	75.498	129.161	-105.691	1.453
3900	20.958	221.607	201.711	77.594	129.195	-111.871	1.498
4000	20.950	222.137	202.215	79.690	129.226	-118.053	1.542
4100	20.943	222.655	202.707	81.784	129.255	-124.235	1.583
4200	20.936	223.159	203.188	83.878	129.284	-130.418	1.622
4300	20.929	223.652	203.658	85.971	129.314	-136.602	1.659
4400	20.923	224.133	204.118	88.064	129.347	-142.786	1.695
4500	20.918	224.603	204.568	90.156	129.384	-148.972	1.729
4600	20.912	225.063	205.009	92.247	129.426	-155.158	1.762
4700	20.907	225.512	205.440	94.338	129.474	-161.345	1.793
4800	20.903	225.952	205.863	96.429	129.530	-167.533	1.823
4900	20.898	226.383	206.278	98.519	129.594	-173.723	1.852
5000	20.894	226.806	206.684	100.609	129.667	-179.914	1.880
5100	20.890	227.219	207.082	102.698	129.750	-186.106	1.906
5200	20.886	227.625	207.474	104.787	129.844	-192.300	1.932
5300	20.883	228.023	207.858	106.875	129.950	-198.496	1.956
5400	20.879	228.413	208.235	108.963	130.068	-204.694	1.980
5500	20.876	228.796	208.605	111.051	130.199	-210.895	2.003
5600	20.873	229.172	208.969	113.138	130.343	-217.098	2.025
5700	20.870	229.542	209.327	115.226	130.501	-223.304	2.046
5800	20.867	229.905	209.678	117.312	130.673	-229.512	2.067
5900	20.865	230.261	210.024	119.399	130.859	-235.724	2.087
6000	20.862	230.612	210.364	121.485	131.059	-241.939	2.106

PREVIOUS: June 1972 (1 atm) CURRENT: June 1982 (1 bar)

Table A-1. Calculation for Monatomic Specie: Cl (Continued).

Cl b. MONATOMIC GAS

T(K)	Cp	S0	-(G0-H0298)/T	H0-H0298	T(K)	Cp	S0	-(G0-H0298)/T	H0-H0298
0	.000	.000	1.0e99	-6.272	10600	21.225	242.506	221.970	217.682
100	20.788	142.174	184.107	-4.193	10800	21.305	242.904	222.354	221.935
200	21.081	156.636	167.163	-2.105	11000	21.396	243.296	222.731	226.205
300	21.856	165.326	165.191	.040	11200	21.501	243.682	223.102	230.494
400	22.470	171.705	166.056	2.260	11400	21.620	244.064	223.467	234.806
500	22.745	176.755	167.709	4.523	11600	21.754	244.441	223.825	239.143
600	22.781	180.907	169.573	6.801	11800	21.904	244.814	224.177	243.508
700	22.691	184.413	171.449	9.075	12000	22.072	245.183	224.525	247.906
800	22.547	187.434	173.263	11.337	12200	22.259	245.550	224.866	252.339
900	22.387	190.081	174.988	13.584	12400	22.466	245.913	225.203	256.811
1000	22.231	192.431	176.617	15.815	12600	22.694	246.275	225.534	261.327
1100	22.087	194.543	178.152	18.030	12800	22.945	246.634	225.861	265.890
1200	21.957	196.459	179.599	20.232	13000	23.219	246.992	226.184	270.506
1300	21.841	198.212	180.964	22.422	13200	23.517	247.348	226.502	275.179
1400	21.740	199.827	182.255	24.601	13400	23.841	247.704	226.815	279.915
1500	21.650	201.324	183.477	26.770	13600	24.191	248.060	227.125	284.717
1600	21.572	202.718	184.636	28.931	13800	24.568	248.416	227.431	289.593
1700	21.502	204.024	185.739	31.085	14000	24.972	248.772	227.733	294.546
1800	21.441	205.251	186.789	33.232	14200	25.406	249.130	228.032	299.584
1900	21.387	206.409	187.791	35.374	14400	25.868	249.488	228.328	304.710
2000	21.339	207.505	188.750	37.510	14600	26.360	249.848	228.620	309.933
2100	21.297	208.545	189.668	39.642	14800	26.882	250.211	228.909	315.257
2200	21.259	209.535	190.549	41.769	15000	27.434	250.575	229.196	320.688
2300	21.225	210.479	191.395	43.894	15200	28.017	250.942	229.480	326.232
2400	21.194	211.382	192.209	46.014	15400	28.629	251.312	229.761	331.896
2500	21.166	212.246	192.993	48.132	15600	29.271	251.686	230.039	337.686
2600	21.141	213.076	193.750	50.248	15800	29.943	252.063	230.316	343.607
2700	21.119	213.873	194.480	52.361	16000	30.645	252.444	230.590	349.665
2800	21.098	214.641	195.187	54.472	16200	31.374	252.829	230.862	355.867
2900	21.079	215.381	195.871	56.580	16400	32.132	253.219	231.132	362.217
3000	21.062	216.095	196.533	58.687	16600	32.916	253.613	231.401	368.721
3100	21.046	216.786	197.175	60.793	16800	33.727	254.012	231.668	375.385
3200	21.032	217.454	197.798	62.897	17000	34.562	254.416	231.933	382.214
3300	21.018	218.101	198.404	64.999	17200	35.420	254.825	232.197	389.211
3400	21.006	218.728	198.992	67.100	17400	36.300	255.240	232.459	396.383
3500	20.995	219.337	199.565	69.200	17600	37.201	255.660	232.721	403.733
3600	20.984	219.928	200.123	71.299	17800	38.119	256.085	232.981	411.264
3700	20.975	220.503	200.666	73.397	18000	39.055	256.517	233.240	418.982
3800	20.966	221.062	201.195	75.494	18200	40.005	256.953	233.498	426.887
3900	20.957	221.606	201.711	77.591	18400	40.967	257.396	233.755	434.984
4000	20.949	222.137	202.216	79.686	18600	41.940	257.844	234.012	443.275
4100	20.942	222.654	202.708	81.780	18800	42.921	258.298	234.268	451.761
4200	20.935	223.159	203.189	83.874	19000	43.908	258.757	234.523	460.444
4300	20.929	223.651	203.659	85.968	19200	44.899	259.222	234.778	469.325
4400	20.923	224.132	204.119	88.060	19400	45.890	259.692	235.032	478.404
4500	20.917	224.603	204.569	90.152	19600	46.880	260.168	235.287	487.681
4600	20.912	225.062	205.009	92.244	19800	47.866	260.649	235.540	497.155
4700	20.907	225.512	205.441	94.334	20000	48.845	261.135	235.794	506.826
4800	20.902	225.952	205.863	96.425	20200	49.816	261.626	236.047	516.693
4900	20.898	226.383	206.278	98.515	20400	50.776	262.122	236.300	526.752
5000	20.894	226.805	206.684	100.605	20600	51.721	262.622	236.553	537.002
5100	20.890	227.219	207.083	102.694	20800	52.651	263.126	236.807	547.440
5200	20.886	227.624	207.474	104.782	21000	53.562	263.634	237.060	558.061
5300	20.882	228.022	207.858	106.871	21200	54.453	264.146	237.313	568.863
5400	20.879	228.413	208.235	108.959	21400	55.321	264.661	237.566	579.841
5500	20.876	228.796	208.605	111.047	21600	56.165	265.180	237.819	590.990
5600	20.873	229.172	208.969	113.134	21800	56.982	265.701	238.073	602.305
5700	20.870	229.541	209.327	115.221	22000	57.770	266.225	238.326	613.781
5800	20.867	229.904	209.679	117.308	22200	58.529	266.752	238.580	625.411
5900	20.865	230.261	210.024	119.395	22400	59.256	267.280	238.834	637.190
6000	20.862	230.611	210.365	121.481	22600	59.950	267.810	239.088	649.112
6200	20.858	231.295	211.029	125.653	22800	60.610	268.341	239.342	661.168
6400	20.854	231.958	211.673	129.824	23000	61.235	268.873	239.597	673.353
6600	20.851	232.599	212.297	133.995	23200	61.823	269.406	239.851	685.660
6800	20.848	233.222	212.903	138.165	23400	62.375	269.939	240.106	698.080
7000	20.846	233.826	213.493	142.334	23600	62.888	270.472	240.361	710.607
7200	20.844	234.413	214.066	146.503	23800	63.364	271.004	240.616	723.233
7400	20.844	234.984	214.623	150.672	24000	63.801	271.536	240.872	735.950
7600	20.844	235.540	215.166	154.841	24200	64.199	272.068	241.128	748.751
7800	20.845	236.082	215.696	159.009	24400	64.558	272.598	241.383	761.627
8000	20.848	236.609	216.212	163.179	24600	64.878	273.126	241.639	774.571
8200	20.853	237.124	216.716	167.349	24800	65.160	273.652	241.895	787.575
8400	20.859	237.627	217.208	171.520	25000	65.403	274.177	242.151	800.632
8600	20.869	238.118	217.688	175.693	25500	65.847	275.477	242.792	833.455
8800	20.881	238.598	218.158	179.868	26000	66.063	276.758	243.433	866.441
9000	20.896	239.067	218.618	184.045	26500	66.065	278.016	244.074	899.482
9200	20.915	239.527	219.067	188.226	27000	65.868	279.250	244.714	932.473
9400	20.939	239.977	219.507	192.412	27500	65.489	280.455	245.353	965.320
9600	20.969	240.418	219.938	196.602	28000	64.948	281.631	245.990	997.935
9800	21.004	240.850	220.361	200.800	28500	64.263	282.774	246.625	1030.244
10000	21.047	241.275	220.775	205.005	29000	63.455	283.885	247.258	1062.178
10200	21.097	241.692	221.181	209.219	29500	62.542	284.962	247.888	1093.681
10400	21.156	242.103	221.579	213.444	30000	61.542	286.005	248.515	1124.705

Table A-2. JANAF Table for Diatomic Specie: CF.

a. Fluoromethylidyne (CF) $C_1F_1(g)$

Enthalpy Reference Temperature = T_r = 298.15 K **Standard State Pressure = p° = 0.1 MPa**

	J K⁻¹mol⁻¹			kJ mol⁻¹			
T/K	$C_p°$	S°	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	Log K_f
0	0.	0.	INFINITE	-9.082	251.605	251.605	INFINITE
100	31.017	180.140	239.625	-5.948	253.226	243.826	-127.361
200	29.778	201.126	215.766	-2.928	254.455	233.912	-61.092
250	29.792	207.766	213.526	-1.440	254.896	228.723	-47.789
298.15	30.060	213.033	213.033	0.	255.224	223.650	-39.183
300	30.074	213.219	213.034	0.056	255.235	223.455	-38.907
350	30.537	217.888	213.402	1.570	255.484	218.137	-32.555
400	31.094	222.002	214.224	3.111	255.658	212.789	-27.787
450	31.681	225.698	215.297	4.680	255.765	207.423	-24.077
500	32.253	229.066	216.508	6.279	255.816	202.049	-21.108
600	33.280	235.040	219.111	9.557	255.779	191.296	-16.654
700	34.116	240.235	221.766	12.928	255.602	180.561	-13.474
800	34.780	244.836	224.368	16.374	255.322	169.859	-11.091
900	35.305	248.964	226.875	19.880	254.966	159.197	-9.240
1000	35.725	252.706	229.274	23.432	254.550	148.577	-7.761
1100	36.064	256.127	231.562	27.022	254.086	138.002	-6.553
1200	36.343	259.278	233.742	30.643	253.583	127.471	-5.549
1300	36.576	262.196	235.820	34.289	253.046	116.983	-4.700
1400	36.773	264.914	237.802	37.957	252.479	106.538	-3.975
1500	36.942	267.457	239.695	41.643	251.885	96.134	-3.348
1600	37.088	269.846	241.506	45.344	251.267	85.771	-2.800
1700	37.218	272.098	243.240	49.060	250.628	75.447	-2.318
1800	37.333	274.229	244.903	52.787	249.969	65.161	-1.891
1900	37.436	276.250	246.500	56.526	249.292	54.913	-1.510
2000	37.530	278.173	248.036	60.274	248.601	44.700	-1.167
2100	37.617	280.006	249.515	64.032	247.896	34.522	-0.859
2200	37.697	281.758	250.941	67.797	247.180	24.378	-0.579
2300	37.771	283.435	252.318	71.571	246.456	14.267	-0.324
2400	37.841	285.044	253.648	75.352	245.725	4.187	-0.091
2500	37.907	286.591	254.935	79.139	244.990	-5.861	0.122
2600	37.970	288.079	256.181	82.933	244.253	-15.881	0.319
2700	38.030	289.513	257.389	86.733	243.516	-25.872	0.501
2800	38.089	290.897	258.561	90.539	242.780	-35.836	0.669
2900	38.145	292.234	259.700	94.351	242.047	-45.774	0.824
3000	38.200	293.528	260.806	98.168	241.319	-55.686	0.970
3100	38.254	294.782	261.882	101.991	240.597	-65.574	1.105
3200	38.307	295.997	262.929	105.819	239.882	-75.439	1.231
3300	38.360	297.177	263.949	109.652	239.175	-85.282	1.350
3400	38.413	298.323	264.943	113.491	238.477	-95.104	1.461
3500	38.466	299.437	265.913	117.335	237.789	-104.905	1.566
3600	38.519	300.521	266.859	121.184	237.110	-114.686	1.664
3700	38.572	301.578	267.783	125.038	236.442	-124.449	1.757
3800	38.627	302.607	268.686	128.898	235.785	-134.195	1.845
3900	38.682	303.611	269.569	132.764	235.139	-143.922	1.928
4000	38.738	304.591	270.432	136.635	234.505	-153.634	2.006
4100	38.796	305.548	271.277	140.511	233.882	-163.330	2.081
4200	38.855	306.484	272.104	144.394	233.270	-173.010	2.152
4300	38.915	307.399	272.915	148.282	232.670	-182.676	2.219
4400	38.977	308.294	273.709	152.177	232.081	-192.329	2.283
4500	39.040	309.171	274.487	156.078	231.504	-201.968	2.344
4600	39.105	310.030	275.250	159.985	230.938	-211.594	2.403
4700	39.172	310.871	275.999	163.899	230.383	-221.209	2.458
4800	39.241	311.697	276.734	167.820	229.839	-230.811	2.512
4900	39.311	312.507	277.456	171.747	229.306	-240.403	2.563
5000	39.383	313.301	278.165	175.682	228.784	-249.983	2.612
5100	39.457	314.082	278.862	179.624	228.272	-259.553	2.658
5200	39.532	314.849	279.546	183.573	227.771	-269.114	2.703
5300	39.610	315.603	280.220	187.530	227.279	-278.664	2.746
5400	39.689	316.344	280.882	191.495	226.798	-288.206	2.788
5500	39.769	317.073	281.533	195.468	226.327	-297.739	2.828
5600	39.851	317.790	282.174	199.449	225.865	-307.263	2.866
5700	39.935	318.496	282.805	203.438	225.413	-316.779	2.903
5800	40.021	319.192	283.427	207.436	224.970	-326.288	2.939
5900	40.107	319.876	284.039	211.443	224.536	-335.788	2.973
6000	40.196	320.551	284.642	215.458	224.111	-345.282	3.006

PREVIOUS: June 1970 (1 atm) CURRENT: June 1970 (1 bar)

Table A-2. Calculation for Diatomic Specie: CF (Continued).

CF b. DIATOMIC GAS

T(K)	Cp	S0	-(G0-H0298)/T	H0-H0298	T(K)	Cp	S0	-(G0-H0298)/T	H0-H0298
0	.000	.000	1.0e99	-9.088	10600	44.690	344.585	305.838	410.720
100	31.017	180.140	239.625	-5.948	10800	44.869	345.422	306.563	419.676
200	29.778	201.125	215.765	-2.928	11000	45.044	346.247	307.277	428.668
300	30.074	213.219	213.033	.056	11200	45.216	347.060	307.980	437.694
400	31.094	222.001	214.224	3.111	11400	45.385	347.862	308.673	446.754
500	32.253	229.065	216.507	6.279	11600	45.550	348.653	309.355	455.847
600	33.280	235.039	219.111	9.557	11800	45.711	349.433	310.028	464.973
700	34.116	240.234	221.765	12.928	12000	45.869	350.202	310.691	474.131
800	34.780	244.835	224.367	16.374	12200	46.024	350.962	311.345	483.321
900	35.305	248.963	226.874	19.880	12400	46.175	351.711	311.990	492.541
1000	35.725	252.705	229.273	23.432	12600	46.323	352.451	312.627	501.791
1100	36.064	256.127	231.561	27.022	12800	46.467	353.182	313.255	511.070
1200	36.343	259.277	233.741	30.643	13000	46.608	353.903	313.874	520.377
1300	36.576	262.195	235.819	34.289	13200	46.745	354.616	314.486	529.713
1400	36.773	264.913	237.801	37.957	13400	46.879	355.320	315.091	539.075
1500	36.942	267.456	239.695	41.643	13600	47.009	356.016	315.687	548.464
1600	37.088	269.845	241.505	45.344	13800	47.137	356.703	316.277	557.879
1700	37.218	272.098	243.239	49.060	14000	47.260	357.382	316.859	567.318
1800	37.333	274.228	244.902	52.787	14200	47.381	358.053	317.435	576.783
1900	37.436	276.250	246.499	56.526	14400	47.499	358.717	318.003	586.271
2000	37.530	278.172	248.035	60.274	14600	47.613	359.373	318.566	595.782
2100	37.617	280.006	249.514	64.032	14800	47.725	360.021	319.121	605.316
2200	37.697	281.757	250.940	67.797	15000	47.833	360.662	319.671	614.872
2300	37.771	283.435	252.317	71.571	15200	47.939	361.297	320.215	624.449
2400	37.841	285.044	253.647	75.352	15400	48.041	361.924	320.752	634.047
2500	37.907	286.590	254.934	79.139	15600	48.141	362.545	321.284	643.665
2600	37.970	288.078	256.181	82.933	15800	48.239	363.158	321.810	653.303
2700	38.030	289.512	257.389	86.733	16000	48.333	363.766	322.331	662.961
2800	38.089	290.896	258.561	90.539	16200	48.426	364.367	322.846	672.637
2900	38.145	292.234	259.699	94.351	16400	48.515	364.962	323.356	682.331
3000	38.200	293.528	260.805	98.168	16600	48.603	365.550	323.861	692.043
3100	38.254	294.781	261.881	101.991	16800	48.688	366.133	324.361	701.772
3200	38.307	295.997	262.928	105.819	17000	48.771	366.709	324.856	711.518
3300	38.360	297.176	263.948	109.652	17200	48.852	367.280	325.346	721.280
3400	38.413	298.322	264.943	113.491	17400	48.930	367.846	325.831	731.058
3500	38.466	299.436	265.912	117.335	17600	49.007	368.405	326.311	740.852
3600	38.519	300.521	266.859	121.184	17800	49.082	368.959	326.787	750.661
3700	38.572	301.577	267.783	125.038	18000	49.154	369.508	327.259	760.484
3800	38.627	302.606	268.686	128.898	18200	49.226	370.052	327.726	770.322
3900	38.682	303.610	269.568	132.764	18400	49.295	370.590	328.189	780.174
4000	38.738	304.590	270.432	136.635	18600	49.363	371.123	328.648	790.040
4100	38.796	305.548	271.276	140.511	18800	49.429	371.652	329.103	799.919
4200	38.855	306.483	272.104	144.394	19000	49.493	372.175	329.553	809.812
4300	38.915	307.398	272.914	148.282	19200	49.556	372.694	330.000	819.716
4400	38.977	308.293	273.708	152.177	19400	49.618	373.208	330.443	829.634
4500	39.040	309.170	274.486	156.078	19600	49.678	373.717	330.882	839.564
4600	39.105	310.029	275.249	159.985	19800	49.737	374.221	331.317	849.505
4700	39.172	310.871	275.998	163.899	20000	49.795	374.722	331.749	859.458
4800	39.241	311.696	276.734	167.820	20200	49.852	375.217	332.177	869.423
4900	39.311	312.506	277.455	171.747	20400	49.908	375.709	332.601	879.399
5000	39.383	313.301	278.164	175.682	20600	49.962	376.196	333.022	889.386
5100	39.457	314.081	278.861	179.624	20800	50.016	376.679	333.439	899.384
5200	39.532	314.848	279.546	183.573	21000	50.068	377.158	333.853	909.392
5300	39.610	315.602	280.219	187.530	21200	50.120	377.633	334.264	919.411
5400	39.689	316.343	280.881	191.495	21400	50.171	378.104	334.672	929.440
5500	39.769	317.072	281.532	195.468	21600	50.220	378.570	335.076	939.479
5600	39.851	317.789	282.174	199.449	21800	50.270	379.034	335.477	949.528
5700	39.935	318.496	282.805	203.438	22000	50.318	379.493	335.875	959.587
5800	40.021	319.191	283.426	207.436	22200	50.366	379.948	336.270	969.656
5900	40.107	319.876	284.038	211.443	22400	50.413	380.400	336.662	979.733
6000	40.196	320.551	284.641	215.458	22600	50.459	380.849	337.051	989.821
6200	40.376	321.871	285.821	223.515	22800	50.505	381.294	337.437	999.917
6400	40.561	323.156	286.967	231.608	23000	50.550	381.735	337.821	1010.023
6600	40.750	324.407	288.083	239.740	23200	50.595	382.173	338.201	1020.137
6800	40.944	325.627	289.169	247.909	23400	50.640	382.607	338.579	1030.261
7000	41.140	326.816	290.228	256.117	23600	50.684	383.038	338.954	1040.393
7200	41.339	327.978	291.261	264.365	23800	50.727	383.466	339.326	1050.534
7400	41.539	329.113	292.268	272.653	24000	50.770	383.891	339.696	1060.684
7600	41.742	330.224	293.253	280.981	24200	50.813	384.312	340.063	1070.842
7800	41.945	331.311	294.215	289.349	24400	50.855	384.731	340.427	1081.009
8000	42.149	332.375	295.155	297.759	24600	50.897	385.146	340.789	1091.184
8200	42.353	333.419	296.076	306.209	24800	50.939	385.558	341.148	1101.368
8400	42.557	334.442	296.977	314.700	25000	50.980	385.968	341.505	1111.560
8600	42.760	335.445	297.860	323.232	25500	51.083	386.978	342.387	1137.076
8800	42.962	336.431	298.726	331.804	26000	51.185	387.971	343.254	1162.643
9000	43.163	337.398	299.574	340.416	26500	51.286	388.947	344.107	1188.261
9200	43.362	338.349	300.407	349.069	27000	51.386	389.907	344.946	1213.929
9400	43.559	339.284	301.224	357.761	27500	51.486	390.851	345.772	1239.647
9600	43.754	340.203	302.027	366.492	28000	51.586	391.779	346.586	1265.415
9800	43.947	341.107	302.815	375.262	28500	51.686	392.693	347.387	1291.232
10000	44.137	341.997	303.590	384.071	29000	51.786	393.593	348.176	1317.100
10200	44.324	342.873	304.352	392.917	29500	51.886	394.479	348.953	1343.018
10400	44.509	343.735	305.101	401.800	30000	51.987	395.352	349.719	1368.986

Table A-3. JANAF Table for Linear Polyatomic Specie: C_2Cl_2.

a. Dichloroethyne (C_2Cl_2) $C_2Cl_2(g)$

Enthalpy Reference Temperature = T_r = 298.15 K **Standard State Pressure = p° = 0.1 MPa**

	J K^{-1}mol^{-1}			kJ mol^{-1}			
T/K	$C_p°$	$S° - [G° - H°(T_r)]/T$		$H° - H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	Log K_f
0	0.	0.	INFINITE	-14.565	206.336	206.336	INFINITE
100	42.627	212.575	324.555	-11.198	206.672	204.506	-106.823
200	57.837	247.336	277.809	-6.095	208.085	201.843	-52.716
250	62.360	260.755	273.089	-3.084	208.886	200.190	-41.827
298.15	65.573	272.027	272.027	0.	209.618	198.448	-34.767
300	65.680	272.433	272.028	0.121	209.645	198.378	-34.541
350	68.213	282.756	272.837	3.471	210.335	196.445	-29.318
400	70.218	292.000	274.665	6.934	210.942	194.418	-25.388
450	71.861	300.368	277.063	10.487	211.463	192.320	-22.324
500	73.250	308.013	279.782	14.116	211.900	190.169	-19.867
600	75.515	321.577	285.646	21.559	212.554	185.757	-16.172
700	77.312	333.358	291.639	29.203	212.981	181.255	-13.525
800	78.775	343.780	297.517	37.010	213.246	176.703	-11.538
900	79.977	353.130	303.186	44.950	213.396	172.125	-9.990
1000	80.970	361.610	308.611	52.999	213.462	167.535	-8.751
1100	81.794	369.367	313.787	61.138	213.464	162.942	-7.737
1200	82.480	376.514	318.720	69.353	213.414	158.351	-6.893
1300	83.055	383.139	323.424	77.630	213.322	153.765	-6.178
1400	83.539	389.312	327.912	85.961	213.191	149.189	-5.566
1500	83.950	395.090	332.200	94.336	213.026	144.623	-5.036
1600	84.300	400.520	336.302	102.749	212.829	140.069	-4.573
1700	84.600	405.640	340.232	111.194	212.602	135.528	-4.164
1800	84.859	410.483	344.001	119.667	212.344	131.002	-3.802
1900	85.084	415.077	347.622	128.165	212.056	126.490	-3.477
2000	85.280	419.447	351.105	136.683	211.738	121.995	-3.186
2100	85.452	423.612	354.459	145.220	211.389	117.516	-2.923
2200	85.604	427.590	357.694	153.773	211.008	113.055	-2.684
2300	85.738	431.399	360.816	162.340	210.594	108.611	-2.467
2400	85.857	435.050	363.834	170.920	210.146	104.187	-2.268
2500	85.964	438.557	366.753	179.511	209.662	99.782	-2.085
2600	86.059	441.931	369.580	188.112	209.142	95.397	-1.917
2700	86.144	445.180	372.320	196.723	208.583	91.033	-1.761
2800	86.222	448.315	374.978	205.341	207.987	86.689	-1.617
2900	86.291	451.341	377.560	213.967	207.351	82.368	-1.484
3000	86.355	454.268	380.068	222.599	206.677	78.070	-1.359
3100	86.412	457.100	382.508	231.238	205.963	73.795	-1.243
3200	86.465	459.845	384.882	239.881	205.211	69.543	-1.135
3300	86.513	462.506	387.194	248.530	204.421	65.316	-1 034
3400	86.557	465.090	389.447	257.184	203.595	61.113	-0.939
3500	86.598	467.599	391.644	265.842	202.734	56.935	-0.850
3600	86.635	470.039	393.788	274.503	201.840	52.782	-0.766
3700	86.670	472.413	395.881	283.169	200.915	48.654	-0.687
3800	86.702	474.725	397.926	291.837	199.961	44 551	-0.612
3900	86.731	476.978	399.924	300.509	198.981	40.474	-0.542
4000	86.759	479.174	401.878	309.183	197.978	36.423	-0.476
4100	86.784	481.317	403.790	317.861	196.953	32.396	-0.413
4200	86.808	483.408	405.660	326.540	195.909	28.395	-0.353
4300	86.830	485.451	407.492	335.222	194.850	24.420	-0.297
4400	86.851	487.447	409.287	343.906	193.776	20.468	-0.243
4500	86.870	489.399	411.046	352.592	192.692	16.542	-0.192
4600	86.888	491.309	412.770	361.280	191.599	12.639	-0.144
4700	86.906	493.178	414.461	369.970	190.500	8.761	-0.097
4800	86.922	495.008	416.120	378.661	189.397	4.906	-0.053
4900	86.937	496.800	417.748	387.354	188.291	1.074	-0.011
5000	86.951	498.557	419.347	396.048	187.185	-2.736	0.029
5100	86.964	500.279	420.917	404.744	186.079	-6.523	0 067
5200	86.977	501.967	422.459	413.441	184.977	-10.289	0.103
5300	86.989	503.624	423.975	422.140	183.878	-14.034	0.138
5400	87.000	505.250	425.465	430.839	182.785	-17.758	0.172
5500	87.011	506.847	426.930	439.540	181.698	-21.461	0.204
5600	87.021	508.415	428.372	448.241	180.617	-25.146	0.235
5700	87.031	509.955	429.789	456.944	179.545	-28.811	0.264
5800	87.040	511.469	431.185	465.647	178.481	-32.456	0.292
5900	87.048	512.957	432.558	474.352	177.427	-36.084	0.319
6000	87.057	514.420	433.910	483.057	176.381	-39.695	0.346

PREVIOUS: December 1968 (1 atm) CURRENT: December 1968 (1 bar)

Table A-3. Calculation for Linear Polyatomic Specie: C_2Cl_2 (Continued).

C2Cl2 b. LINEAR POLYATOMIC GAS

T(K)	Cp	S0	-(G0-H0298)/T	H0-H0298
0	.000	.000	1.0e99	-14.565
100	42.627	212.574	324.554	-11.198
200	57.837	247.335	277.808	-6.095
300	65.680	272.432	272.027	.121
400	70.218	291.999	274.664	6.934
500	73.250	308.012	279.781	14.116
600	75.515	321.576	285.645	21.559
700	77.312	333.357	291.638	29.203
800	78.775	343.779	297.516	37.010
900	79.977	353.129	303.185	44.950
1000	80.970	361.609	308.610	52.999
1100	81.794	369.366	313.786	61.138
1200	82.480	376.513	318.719	69.353
1300	83.055	383.138	323.423	77.630
1400	83.539	389.312	327.911	85.961
1500	83.950	395.090	332.199	94.336
1600	84.300	400.519	336.301	102.749
1700	84.600	405.639	340.231	111.194
1800	84.859	410.482	344.000	119.667
1900	85.084	415.076	347.621	128.165
2000	85.280	419.446	351.104	136.683
2100	85.452	423.611	354.458	145.220
2200	85.604	427.590	357.693	153.773
2300	85.738	431.398	360.815	162.340
2400	85.857	435.049	363.833	170.920
2500	85.964	438.556	366.752	179.511
2600	86.059	441.930	369.579	188.112
2700	86.144	445.179	372.319	196.723
2800	86.222	448.314	374.978	205.341
2900	86.291	451.341	377.559	213.967
3000	86.355	454.267	380.067	222.599
3100	86.412	457.100	382.507	231.237
3200	86.465	459.844	384.881	239.881
3300	86.513	462.505	387.193	248.530
3400	86.557	465.089	389.446	257.184
3500	86.598	467.598	391.644	265.842
3600	86.635	470.038	393.787	274.503
3700	86.670	472.413	395.881	283.169
3800	86.702	474.724	397.925	291.837
3900	86.731	476.977	399.923	300.509
4000	86.759	479.173	401.877	309.183
4100	86.784	481.316	403.789	317.860
4200	86.808	483.407	405.660	326.540
4300	86.830	485.450	407.491	335.222
4400	86.851	487.447	409.286	343.906
4500	86.870	489.399	411.045	352.592
4600	86.888	491.308	412.769	361.280
4700	86.906	493.177	414.460	369.970
4800	86.922	495.007	416.119	378.661
4900	86.937	496.799	417.747	387.354
5000	86.951	498.556	419.346	396.048
5100	86.964	500.278	420.916	404.744
5200	86.977	501.966	422.458	413.441
5300	86.989	503.623	423.974	422.140
5400	87.000	505.249	425.464	430.839
5500	87.011	506.846	426.930	439.540
5600	87.021	508.414	428.371	448.241
5700	87.031	509.954	429.789	456.944
5800	87.040	511.468	431.184	465.647
5900	87.048	512.956	432.557	474.352
6000	87.057	514.419	433.909	483.057
6200	87.072	517.274	436.553	500.470
6400	87.086	520.038	439.119	517.886
6600	87.099	522.718	441.612	535.304
6800	87.110	525.319	444.036	552.725
7000	87.121	527.844	446.394	570.148
7200	87.131	530.298	448.691	587.574
7400	87.140	532.686	450.929	605.001
7600	87.148	535.010	453.111	622.429
7800	87.156	537.274	455.240	639.860
8000	87.163	539.480	457.319	657.292
8200	87.170	541.633	459.349	674.725
8400	87.176	543.733	461.333	692.160
8600	87.182	545.785	463.274	709.595
8800	87.187	547.789	465.172	727.032
9000	87.192	549.748	467.029	744.470
9200	87.197	551.665	468.849	761.909
9400	87.201	553.540	470.631	779.349
9600	87.205	555.376	472.377	796.789
9800	87.209	557.174	474.089	814.231
10000	87.213	558.936	475.769	831.673
10200	87.216	560.663	477.416	849.116
10400	87.219	562.357	479.034	866.559
10600	87.222	564.018	480.622	884.004
10800	87.225	565.649	482.181	901.448
11000	87.228	567.249	483.713	918.894
11200	87.231	568.821	485.219	936.340
11400	87.233	570.365	486.699	953.786
11600	87.235	571.882	488.155	971.233
11800	87.238	573.373	489.587	988.680
12000	87.240	574.839	490.995	1006.128
12200	87.242	576.281	492.382	1023.576
12400	87.244	577.700	493.746	1041.024
12600	87.245	579.096	495.090	1058.473
12800	87.247	580.470	496.414	1075.923
13000	87.249	581.823	497.717	1093.372
13200	87.250	583.155	499.002	1110.822
13400	87.252	584.467	500.267	1128.272
13600	87.253	585.759	501.515	1145.723
13800	87.255	587.033	502.745	1163.174
14000	87.256	588.289	503.958	1180.625
14200	87.257	589.526	505.155	1198.076
14400	87.258	590.747	506.335	1215.528
14600	87.260	591.950	507.500	1232.979
14800	87.261	593.138	508.649	1250.431
15000	87.262	594.309	509.783	1267.884
15200	87.263	595.465	510.903	1285.336
15400	87.264	596.606	512.009	1302.789
15600	87.265	597.732	513.101	1320.242
15800	87.266	598.843	514.179	1337.695
16000	87.267	599.941	515.244	1355.148
16200	87.267	601.025	516.297	1372.601
16400	87.268	602.096	517.336	1390.055
16600	87.269	603.154	518.364	1407.509
16800	87.270	604.199	519.380	1424.962
17000	87.271	605.232	520.384	1442.417
17200	87.271	606.252	521.376	1459.871
17400	87.272	607.261	522.357	1477.325
17600	87.273	608.259	523.328	1494.779
17800	87.273	609.245	524.288	1512.234
18000	87.274	610.220	525.237	1529.689
18200	87.274	611.184	526.176	1547.144
18400	87.275	612.138	527.106	1564.599
18600	87.276	613.082	528.025	1582.054
18800	87.276	614.015	528.935	1599.509
19000	87.277	614.939	529.835	1616.964
19200	87.277	615.853	530.727	1634.419
19400	87.278	616.757	531.609	1651.875
19600	87.278	617.652	532.482	1669.331
19800	87.279	618.538	533.347	1686.786
20000	87.279	619.415	534.203	1704.242
20200	87.280	620.284	535.051	1721.698
20400	87.280	621.144	535.891	1739.154
20600	87.280	621.995	536.723	1756.610
20800	87.281	622.839	537.547	1774.066
21000	87.281	623.674	538.363	1791.522
21200	87.282	624.501	539.172	1808.978
21400	87.282	625.321	539.973	1826.435
21600	87.282	626.133	540.767	1843.891
21800	87.283	626.937	541.554	1861.348
22000	87.283	627.734	542.334	1878.804
22200	87.283	628.524	543.107	1896.261
22400	87.284	629.307	543.873	1913.717
22600	87.284	630.083	544.633	1931.174
22800	87.284	630.852	545.386	1948.631
23000	87.284	631.614	546.132	1966.088
23200	87.285	632.370	546.872	1983.545
23400	87.285	633.119	547.606	2001.002
23600	87.285	633.862	548.334	2018.459
23800	87.286	634.598	549.056	2035.916
24000	87.286	635.329	549.772	2053.373
24200	87.286	636.053	550.482	2070.830
24400	87.286	636.772	551.186	2088.287
24600	87.287	637.484	551.885	2105.745
24800	87.287	638.191	552.578	2123.202
25000	87.287	638.892	553.266	2140.660
25500	87.288	640.621	554.962	2184.303
26000	87.288	642.316	556.625	2227.947
26500	87.289	643.978	558.258	2271.591
27000	87.289	645.610	559.860	2315.236
27500	87.290	647.212	561.434	2358.880
28000	87.290	648.784	562.980	2402.525
28500	87.290	650.329	564.499	2446.170
29000	87.291	651.848	565.992	2489.816
29500	87.291	653.340	567.460	2533.461
30000	87.291	654.807	568.903	2577.107

Table A-4. JANAF Table for Nonlinear Polyatomic Specie: CF_4.

a. Tetrafluoromethane (CF_4) $C_1F_4(g)$

Enthalpy Reference Temperature = T_r = 298.15 K **Standard State Pressure = p° = 0.1 MPa**

	J K⁻¹mol⁻¹			kJ mol⁻¹			
T/K	$C_p°$	S°	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	Log K_f
0	0.	0.	INFINITE	-12.731	-927.229	-927.229	INFINITE
100	34.745	212.363	306.188	-9.383	-929.755	-916.822	478.899
200	47.370	239.882	266.577	-5.339	-931.896	-902.995	235.838
250	54.623	251.239	262.389	-2.788	-932.645	-895.679	187.142
298.15	61.054	261.419	261.419	0.	-933.199	-888.507	155.663
300	61.288	261.798	261.420	0.113	-933.218	-888.229	154.654
350	67.217	271.700	262.189	3.329	-933.651	-880.695	131.437
400	72.400	281.022	263.966	6.822	-933.970	-873.107	114.016
450	76.875	289.815	266.354	10.557	-934.198	-865.485	100.463
500	80.712	298.118	269.120	14.499	-934.351	-857.841	89.618
600	86.781	313.399	275.249	22.890	-934.485	-842.523	73.348
700	91.209	327.127	281.697	31.801	-934.451	-827.197	61.726
800	94.476	339.530	288.164	41.093	-934.298	-811.884	53.011
900	96.927	350.806	294.507	50.669	-934.065	-796.596	46.233
1000	98.797	361.119	300.660	60.459	-933.778	-781.337	40.813
1100	100.249	370.607	306.593	70.415	-933.456	-766.108	36.379
1200	101.394	379.380	312.298	80.499	-933.115	-750.909	32.686
1300	102.312	387.534	317.776	90.686	-932.766	-735.739	29.562
1400	103.057	395.144	323.033	100.956	-932.417	-720.597	26.886
1500	103.669	402.276	328.081	111.293	-932.075	-705.479	24.567
1600	104.178	408.983	332.930	121.686	-931.744	-690.383	22.539
1700	104.605	415.312	337.591	132.126	-931.428	-675.308	20.750
1800	104.966	421.302	342.077	142.605	-931.125	-660.251	19.160
1900	105.275	426.986	346.398	153.117	-930.835	-645.210	17.738
2000	105.540	432.392	350.563	163.658	-930.556	-630.184	16.459
2100	105.770	437.547	354.584	174.224	-930.283	-615.173	15.302
2200	105.970	442.473	358.467	184.811	-930.011	-600.174	14.250
2300	106.146	447.187	362.223	195.417	-929.735	-585.187	13.290
2400	106.301	451.708	365.858	206.040	-929.449	-570.213	12.410
2500	106.438	456.050	369.379	216.677	-929.146	-555.251	11.601
2600	106.560	460.227	372.794	227.327	-928.821	-540.302	10.855
2700	106.669	464.251	376.107	237.988	-928.466	-525.365	10.164
2800	106.767	468.132	379.325	248.660	-928.077	-510.442	9.522
2900	106.855	471.880	382.452	259.342	-927.649	-495.534	8.926
3000	106.935	475.504	385.494	270.031	-927.177	-480.642	8.369
3100	107.007	479.012	388.454	280.728	-926.656	-465.766	7.848
3200	107.073	482.410	391.337	291.432	-926.084	-450.907	7.360
3300	107.132	485.706	394.147	302.143	-925.458	-436.068	6.902
3400	107.187	488.905	396.888	312.859	-924.775	-421.248	6.472
3500	107.237	492.013	399.561	323.580	-924.034	-406.449	6.066
3600	107.283	495.034	402.171	334.306	-923.233	-391.671	5.683
3700	107.326	497.974	404.721	345.036	-922.372	-376.918	5.321
3800	107.365	500.837	407.213	355.771	-921.450	-362.188	4.979
3900	107.401	503.626	409.650	366.509	-920.468	-347.483	4.654
4000	107.435	506.346	412.033	377.251	-919.425	-332.804	4.346
4100	107.466	508.999	414.366	387.996	-918.322	-318.153	4.053
4200	107.495	511.589	416.650	398.744	-917.160	-303.528	3.775
4300	107.522	514.119	418.887	409.495	-915.940	-288.932	3.510
4400	107.547	516.591	421.080	420.249	-914.663	-274.365	3.257
4500	107.571	519.008	423.229	431.005	-913.330	-259.827	3.016
4600	107.593	521.373	425.337	441.763	-911.943	-245.321	2.786
4700	107.614	523.687	427.405	452.523	-910.503	-230.844	2.566
4800	107.633	525.953	429.435	463.285	-909.011	-216.399	2.355
4900	107.651	528.172	431.427	474.050	-907.470	-201.986	2.153
5000	107.669	530.347	433.384	484.816	-905.880	-187.604	1.960
5100	107.685	532.480	435.306	495.583	-904.243	-173.255	1.774
5200	107.700	534.571	437.195	506.353	-902.562	-158.937	1.597
5300	107.714	536.622	439.052	517.123	-900.837	-144.653	1.426
5400	107.728	538.636	440.877	527.895	-899.069	-130.403	1.261
5500	107.741	540.613	442.673	538.669	-897.262	-116.185	1.103
5600	107.753	542.554	444.439	549.444	-895.416	-102.000	0.951
5700	107.765	544.461	446.177	560.219	-893.532	-87.849	0.805
5800	107.776	546.336	447.888	570.997	-891.613	-73.731	0.664
5900	107.786	548.178	449.572	581.775	-889.659	-59.645	0.528
6000	107.796	549.990	451.231	592.554	-887.672	-45.595	0.397

PREVIOUS: June 1969 (1 atm) CURRENT: June 1969 (1 bar)

Table A-4. Calculation for Nonlinear Polyatomic Specie: CF_4 (Continued).

CF4 b. NON-LINEAR POLYATOMIC GAS

T(K)	Cp	S0	-(G0-H0298)/T	H0-H0298	T(K)	Cp	S0	-(G0-H0298)/T	H0-H0298
0	.000	.000	1.0e99	-12.731	10600	107.994	611.402	508.667	1088.996
100	34.745	212.363	306.188	-9.383	10800	107.997	613.421	510.588	1110.595
200	47.370	239.882	266.577	-5.339	11000	108.000	615.403	512.476	1132.195
300	61.287	261.798	261.420	.113	11200	108.004	617.349	514.331	1153.795
400	72.400	281.022	263.966	6.822	11400	108.006	619.261	516.156	1175.396
500	80.711	298.118	269.119	14.499	11600	108.009	621.139	517.950	1196.998
600	86.781	313.399	275.249	22.890	11800	108.012	622.985	519.714	1218.600
700	91.209	327.127	281.697	31.801	12000	108.014	624.801	521.451	1240.202
800	94.476	339.530	288.164	41.093	12200	108.017	626.586	523.159	1261.805
900	96.926	350.806	294.507	50.669	12400	108.019	628.343	524.842	1283.409
1000	98.796	361.119	300.660	60.459	12600	108.021	630.071	526.498	1305.013
1100	100.249	370.606	306.593	70.414	12800	108.023	631.772	528.130	1326.617
1200	101.394	379.380	312.298	80.499	13000	108.025	633.447	529.738	1348.222
1300	102.312	387.534	317.775	90.686	13200	108.027	635.096	531.321	1369.827
1400	103.057	395.144	323.033	100.955	13400	108.029	636.721	532.882	1391.433
1500	103.669	402.276	328.081	111.293	13600	108.030	638.321	534.421	1413.039
1600	104.178	408.983	332.929	121.686	13800	108.032	639.898	535.939	1434.645
1700	104.605	415.312	337.591	132.126	14000	108.034	641.453	537.435	1456.252
1800	104.966	421.302	342.077	142.605	14200	108.035	642.985	538.911	1477.859
1900	105.275	426.985	346.397	153.117	14400	108.037	644.496	540.367	1499.466
2000	105.540	432.392	350.563	163.658	14600	108.038	645.986	541.803	1521.073
2100	105.770	437.547	354.583	174.224	14800	108.039	647.456	543.221	1542.681
2200	105.970	442.472	358.467	184.811	15000	108.041	648.907	544.621	1564.289
2300	106.146	447.187	362.223	195.417	15200	108.042	650.338	546.002	1585.897
2400	106.301	451.708	365.858	206.040	15400	108.043	651.750	547.366	1607.506
2500	106.438	456.050	369.379	216.677	15600	108.044	653.144	548.714	1629.114
2600	106.560	460.227	372.794	227.327	15800	108.045	654.520	550.044	1650.723
2700	106.669	464.251	376.107	237.988	16000	108.046	655.880	551.359	1672.333
2800	106.767	468.132	379.325	248.660	16200	108.047	657.222	552.657	1693.942
2900	106.855	471.880	382.452	259.341	16400	108.048	658.548	553.941	1715.551
3000	106.935	475.504	385.494	270.031	16600	108.049	659.857	555.209	1737.161
3100	107.007	479.011	388.454	280.728	16800	108.050	661.151	556.462	1758.771
3200	107.073	482.410	391.337	291.432	17000	108.051	662.430	557.702	1780.381
3300	107.132	485.706	394.147	302.142	17200	108.052	663.694	558.927	1801.991
3400	107.187	488.905	396.887	312.858	17400	108.053	664.943	560.138	1823.602
3500	107.237	492.012	399.561	323.580	17600	108.053	666.178	561.336	1845.212
3600	107.283	495.034	402.171	334.306	17800	108.054	667.399	562.521	1866.823
3700	107.326	497.974	404.721	345.036	18000	108.055	668.606	563.693	1888.434
3800	107.365	500.837	407.213	355.771	18200	108.056	669.800	564.853	1910.045
3900	107.401	503.626	409.649	366.509	18400	108.056	670.981	566.000	1931.656
4000	107.435	506.346	412.033	377.251	18600	108.057	672.149	567.135	1953.268
4100	107.466	508.999	414.366	387.996	18800	108.058	673.305	568.258	1974.879
4200	107.495	511.589	416.650	398.744	19000	108.058	674.448	569.370	1996.491
4300	107.522	514.119	418.887	409.495	19200	108.059	675.580	570.470	2018.102
4400	107.547	516.591	421.080	420.249	19400	108.059	676.700	571.560	2039.714
4500	107.571	519.008	423.229	431.004	19600	108.060	677.808	572.638	2061.326
4600	107.593	521.373	425.337	441.763	19800	108.060	678.905	573.706	2082.938
4700	107.614	523.687	427.405	452.523	20000	108.061	679.991	574.764	2104.550
4800	107.633	525.953	429.435	463.285	20200	108.062	681.066	575.811	2126.163
4900	107.651	528.172	431.427	474.050	20400	108.062	682.131	576.848	2147.775
5000	107.669	530.347	433.384	484.816	20600	108.063	683.185	577.875	2169.387
5100	107.685	532.479	435.306	495.583	20800	108.063	684.229	578.893	2191.000
5200	107.700	534.571	437.195	506.352	21000	108.063	685.264	579.901	2212.613
5300	107.714	536.622	439.052	517.123	21200	108.064	686.288	580.900	2234.225
5400	107.728	538.636	440.877	527.895	21400	108.064	687.303	581.890	2255.838
5500	107.741	540.613	442.673	538.669	21600	108.065	688.308	582.870	2277.451
5600	107.753	542.554	444.439	549.443	21800	108.065	689.304	583.842	2299.064
5700	107.765	544.461	446.177	560.219	22000	108.066	690.291	584.805	2320.677
5800	107.776	546.336	447.888	570.996	22200	108.066	691.269	585.760	2342.290
5900	107.786	548.178	449.572	581.775	22400	108.066	692.238	586.706	2363.904
6000	107.796	549.990	451.231	592.554	22600	108.067	693.198	587.645	2385.517
6200	107.814	553.525	454.474	614.115	22800	108.067	694.151	588.575	2407.130
6400	107.831	556.948	457.623	635.679	23000	108.067	695.094	589.497	2428.744
6600	107.846	560.266	460.683	657.247	23200	108.068	696.030	590.411	2450.357
6800	107.860	563.486	463.660	678.818	23400	108.068	696.958	591.318	2471.971
7000	107.873	566.613	466.557	700.391	23600	108.068	697.877	592.217	2493.584
7200	107.885	569.652	469.379	721.967	23800	108.069	698.789	593.109	2515.198
7400	107.896	572.608	472.129	743.545	24000	108.069	699.694	593.993	2536.812
7600	107.906	575.485	474.811	765.125	24200	108.069	700.591	594.871	2558.426
7800	107.915	578.288	477.429	786.707	24400	108.070	701.480	595.741	2580.040
8000	107.923	581.021	479.984	808.291	24600	108.070	702.362	596.604	2601.654
8200	107.931	583.686	482.481	829.876	24800	108.070	703.237	597.460	2623.268
8400	107.938	586.287	484.922	851.463	25000	108.070	704.105	598.310	2644.882
8600	107.945	588.827	487.309	873.052	25500	108.071	706.245	600.406	2698.917
8800	107.952	591.308	489.644	894.641	26000	108.072	708.344	602.461	2752.953
9000	107.958	593.734	491.931	916.232	26500	108.072	710.403	604.478	2806.989
9200	107.963	596.107	494.170	937.824	27000	108.073	712.423	606.459	2861.025
9400	107.968	598.429	496.363	959.418	27500	108.073	714.406	608.403	2915.062
9600	107.973	600.702	498.514	981.012	28000	108.074	716.353	610.314	2969.099
9800	107.978	602.929	500.622	1002.607	28500	108.074	718.266	612.191	3023.136
10000	107.982	605.110	502.690	1024.203	29000	108.075	720.146	614.036	3077.173
10200	107.986	607.249	504.719	1045.800	29500	108.075	721.993	615.850	3131.211
10400	107.990	609.345	506.711	1067.397	30000	108.076	723.809	617.635	3185.248

APPENDIX B

NOMINAL REACTIONS

The following list shows the nominal reactions that were solved simultaneously to obtain the equilibrium mixture composition of decomposed CCl_2F_2.

Nominal Reactions

1) $2\ CCl_2F_2 \rightleftarrows CCl_4 + CF_4$
2) $CCl_4 \rightleftarrows C + 2Cl_2$
3) $CF_4 \rightleftarrows C + 2F_2$
4) $2\ CCl_3F \rightleftarrows CCl_2F_2 + CCl_4$
5) $2\ CClF_3 \rightleftarrows CCl_2F_2 + CF_4$
6) $F_2 \rightleftarrows 2F$
7) $Cl_2 \rightleftarrows 2\ Cl$
8) $CCl \rightleftarrows C + Cl$
9) $CF \rightleftarrows C + F$
10) $ClF \rightleftarrows Cl + F$
11) $CF_2 \rightleftarrows C + F_2$
12) $C_2 \rightleftarrows 2\ C$
13) $C_3 \rightleftarrows 3\ C$
14) $C_4 \rightleftarrows 2\ C_2$
15) $C_5 \rightleftarrows C_2 + C_3$
16) $CF_4 \rightleftarrows CF_3 + F$
17) $CCl_2 \rightleftarrows Cl + CCl$
18) $CCl_3 \rightleftarrows Cl + CCl_2$
19) $ClF_3 \rightleftarrows ClF + F_2$
20) $ClF_5 \rightleftarrows ClF_3 + F_2$
21) $C_2Cl_2 \rightleftarrows C_2 + Cl_2$
22) $C_2Cl_4 \rightleftarrows C_2Cl_2 + Cl_2$
23) $C_2Cl_6 \rightleftarrows C_2Cl_4 + Cl_2$
24) $C_2F_2 \rightleftarrows C_2 + F_2$
25) $C_2F_4 \rightleftarrows C_2F_2 + F_2$
26) $C_2F_6 \rightleftarrows C_2F_4 + F_2$
27) $Cl^- \rightleftarrows Cl + e^-$
28) $Cl \rightleftarrows Cl^+ + e^-$
29) $Cl^+ \rightleftarrows Cl^{++} + e^-$
30) $Cl^{++} \rightleftarrows Cl^{+++} + e^-$
31) $Cl^{+++} \rightleftarrows Cl^{++++} + e^-$
32) $F^- \rightleftarrows F + e^-$
33) $F \rightleftarrows F^+ + e^-$
34) $F^+ \rightleftarrows F^{++} + e^-$
35) $F^{++} \rightleftarrows F^{+++} + e^-$
36) $F^{+++} \rightleftarrows F^{++++} + e^-$
37) $C^- \rightleftarrows C + e^-$
38) $C \rightleftarrows C^+ + e^-$
39) $C^+ \rightleftarrows C^{++} + e^-$
40) $C^{++} \rightleftarrows C^{+++} + e^-$

41) $C^{+++} \rightleftarrows C^{++++} + e^-$
42) $C_2^- \rightleftarrows C_2 + e^-$
43) $CF \rightleftarrows CF^+ + e^-$
44) $CF_2 \rightleftarrows CF_2^+ + e^-$
45) $CF_3 \rightleftarrows CF_3^+ + e^-$

High Temperature Reaction Equations

46) $Cl^{++++} \rightleftarrows Cl^{+5} + e^-$
47) $Cl^{+5} \rightleftarrows Cl^{+6} + e^-$
48) $Cl^{+6} \rightleftarrows Cl^{+7} + e^-$
49) $Cl^{+7} \rightleftarrows Cl^{+8} + e^-$
50) $Cl^{+8} \rightleftarrows Cl^{+9} + e^-$
51) $Cl^{+9} \rightleftarrows Cl^{+10} + e^-$
52) $F^{++++} \rightleftarrows F^{+5} + e^-$
53) $F^{+5} \rightleftarrows F^{+6} + e^-$
54) $F^{+6} \rightleftarrows F^{+7} + e^-$
55) $C^{++++} \rightleftarrows C^{+5} + e^-$
56) $C^{+5} \rightleftarrows C^{+6} + e^-$

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